

Data Path : Z:\HPCHEM1\BNA F\Data\BF021016\  
 Data File : BF085000.D  
 Acq On : 10 Feb 2016 18:36  
 Operator : SJ/IZ  
 Sample : H1386-06  
 Misc :  
 ALS Vial : 18 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 S4-B018(22-24)

Integration Parameters: rteint.p  
 Integrator: RTE  
 Smoothing : ON  
 Sampling : 1  
 Start Thrs: 0.2  
 Stop Thrs : 0

Filtering: 5  
 Min Area: 3 % of largest Peak  
 Max Peaks: 100  
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
 Peak separation: 5

Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF020116.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.633	3	4	6	rBV	169748	204997	1.90%	0.162%
2	1.678	6	8	11	rVV	129428	177156	1.64%	0.140%
3	1.747	11	14	31	rVB	2165531	3799506	35.22%	2.997%
4	4.753	274	277	284	rBV	652846	1008022	9.34%	0.795%
5	5.210	314	317	319	rBV	2999843	3521151	32.64%	2.777%
6	6.273	407	410	413	rBV	2372664	3536786	32.79%	2.790%
7	6.387	418	420	423	rBV	2849913	3248647	30.11%	2.562%
8	6.616	438	440	443	rBV	599589	829647	7.69%	0.654%
9	6.776	452	454	457	rVB	2600950	2507910	23.25%	1.978%
10	7.199	488	491	493	rBV	2115957	2400060	22.25%	1.893%
11	7.907	551	553	556	rVB	1085554	1027466	9.52%	0.810%
12	8.193	575	578	584	rBV	131275	172824	1.60%	0.136%
13	8.993	645	648	650	rBV	3981167	3605270	33.42%	2.844%
14	9.130	657	660	664	rVB	186660	270905	2.51%	0.214%
15	9.393	681	683	686	rBV	647645	694191	6.43%	0.548%
16	9.610	698	702	704	rBV2	195700	231203	2.14%	0.182%
17	9.656	704	706	708	rBV	1069618	1008724	9.35%	0.796%
18	10.102	742	745	747	rBV2	125677	197233	1.83%	0.156%
19	10.445	773	775	778	rVB	1907413	1760134	16.32%	1.388%
20	10.582	785	787	789	rBV	152580	213376	1.98%	0.168%
21	10.708	796	798	800	rBV	160831	178120	1.65%	0.140%
22	10.811	805	807	810	rBV	581540	514600	4.77%	0.406%
23	11.131	833	835	838	rBV	604966	835870	7.75%	0.659%
24	11.188	838	840	841	rVV	169575	152071	1.41%	0.120%
25	11.211	841	842	846	rVB	225892	191966	1.78%	0.151%
26	11.371	854	856	860	rVB2	175739	208539	1.93%	0.164%
27	11.588	873	875	877	rBV	188540	171793	1.59%	0.136%
28	11.691	882	884	886	rBV	152290	168673	1.56%	0.133%
29	11.862	896	899	902	rBV2	157784	202029	1.87%	0.159%
30	12.251	930	933	934	rVV	1995592	2360810	21.88%	1.862%
31	12.274	934	935	939	rVB2	78710	142478	1.32%	0.112%
32	12.514	950	956	958	rBV4	60380	131573	1.22%	0.104%
33	12.559	958	960	962	rVB	173515	169480	1.57%	0.134%
34	12.616	962	965	967	rBV	636043	569856	5.28%	0.449%

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35	12.719	972	974	977	rBV	1770525	2052726	19.03%	1.619%
36	12.788	977	980	982	rBV	1491858	1269995	11.77%	1.002%
37	12.971	994	996	998	rVB	3217491	3120473	28.93%	2.461%
38	13.097	1004	1007	1010	rBV4	64413	196450	1.82%	0.155%
39	13.142	1010	1011	1013	rBV	104106	109406	1.01%	0.086%
40	13.177	1013	1014	1019	rVB	136720	179258	1.66%	0.141%
41	13.268	1019	1022	1023	rBV3	126211	191704	1.78%	0.151%
42	13.314	1023	1026	1028	rVB2	362107	555638	5.15%	0.438%
43	13.359	1028	1030	1032	rVB2	112379	109758	1.02%	0.087%
44	13.428	1033	1036	1040	rVB	469046	487956	4.52%	0.385%
45	13.497	1040	1042	1043	rBV2	239285	262981	2.44%	0.207%
46	13.519	1043	1044	1047	rVB2	211552	221597	2.05%	0.175%
47	13.588	1047	1050	1052	rBV4	166000	311585	2.89%	0.246%
48	13.634	1052	1054	1057	rBV2	4592494	6307661	58.47%	4.975%
49	13.679	1057	1058	1060	rVB2	374090	404811	3.75%	0.319%
50	13.714	1060	1061	1063	rVB	650983	597978	5.54%	0.472%
51	13.759	1063	1065	1068	rVB2	844152	1450686	13.45%	1.144%
52	13.874	1072	1075	1076	rBV2	74714	116526	1.08%	0.092%
53	13.919	1076	1079	1080	rBV2	107931	198421	1.84%	0.157%
54	13.954	1080	1082	1083	rBV	606065	611991	5.67%	0.483%
55	14.045	1088	1090	1091	rVV	209210	200276	1.86%	0.158%
56	14.079	1091	1093	1095	rVB	317083	287992	2.67%	0.227%
57	14.217	1103	1105	1107	rBV2	115896	165570	1.53%	0.131%
58	14.274	1107	1110	1118	rVV	6275169	8776544	81.36%	6.923%
59	14.388	1118	1120	1123	rVV3	95905	155978	1.45%	0.123%
60	14.571	1131	1136	1139	rVV4	428565	1099658	10.19%	0.867%
61	14.617	1139	1140	1144	rVB2	147053	188850	1.75%	0.149%
62	14.685	1144	1146	1148	rVB	470658	509091	4.72%	0.402%
63	14.880	1158	1163	1166	rBV2	4097120	8276734	76.72%	6.528%
64	14.925	1166	1167	1168	rVB	216853	153382	1.42%	0.121%
65	15.074	1178	1180	1183	rBV3	76109	192140	1.78%	0.152%
66	15.131	1183	1185	1186	rVV	523916	574894	5.33%	0.453%
67	15.165	1186	1188	1190	rVV2	340871	606283	5.62%	0.478%
68	15.211	1190	1192	1194	rVB2	254855	361040	3.35%	0.285%
69	15.348	1202	1204	1206	rBV	630194	741681	6.88%	0.585%
70	15.451	1210	1213	1218	rVV2	909661	1494804	13.86%	1.179%
71	15.554	1218	1222	1224	rVV	1334715	2481615	23.00%	1.957%

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72	15.600	1224	1226	1229	rVV	3011742	5427206	50.31%	4.281%
73	15.657	1229	1231	1234	rVV	598673	1139396	10.56%	0.899%
74	15.783	1238	1242	1245	rVV	753677	1602762	14.86%	1.264%
75	15.851	1245	1248	1253	rVB4	161716	450813	4.18%	0.356%
76	16.011	1260	1262	1263	rBV	159496	205079	1.90%	0.162%
77	16.045	1263	1265	1268	rVB	195966	308786	2.86%	0.244%
78	16.137	1270	1273	1276	rVB2	214863	438886	4.07%	0.346%
79	16.228	1278	1281	1284	rBV	323625	556202	5.16%	0.439%
80	16.308	1284	1288	1292	rVB3	123407	361438	3.35%	0.285%
81	16.423	1295	1298	1301	rBV	251440	475864	4.41%	0.375%
82	16.480	1301	1303	1306	rVV	271494	510761	4.73%	0.403%
83	16.560	1307	1310	1314	rVV	634690	1575266	14.60%	1.243%
84	16.640	1314	1317	1325	rVB2	385684	1161374	10.77%	0.916%
85	16.948	1335	1344	1350	rBV3	2489751	7485206	69.39%	5.904%
86	17.051	1350	1353	1357	rVV	425790	936290	8.68%	0.739%
87	17.154	1357	1362	1366	rVV	988361	2573310	23.85%	2.030%
88	17.223	1366	1368	1374	rVV4	281468	1068902	9.91%	0.843%
89	17.371	1374	1381	1387	rVV	3790296	10787762	100.00%	8.509%
90	17.486	1387	1391	1392	rVV	152548	356491	3.30%	0.281%
91	17.554	1392	1397	1401	rVV2	1077905	3153859	29.24%	2.488%
92	17.634	1401	1404	1409	rVV	546091	1411529	13.08%	1.113%
93	17.737	1410	1413	1419	rVB2	249730	734019	6.80%	0.579%
94	17.977	1430	1434	1441	rVB	175779	541164	5.02%	0.427%
95	18.457	1471	1476	1483	rBV4	233831	902018	8.36%	0.711%
96	18.606	1484	1489	1497	rVB4	356275	1179885	10.94%	0.931%

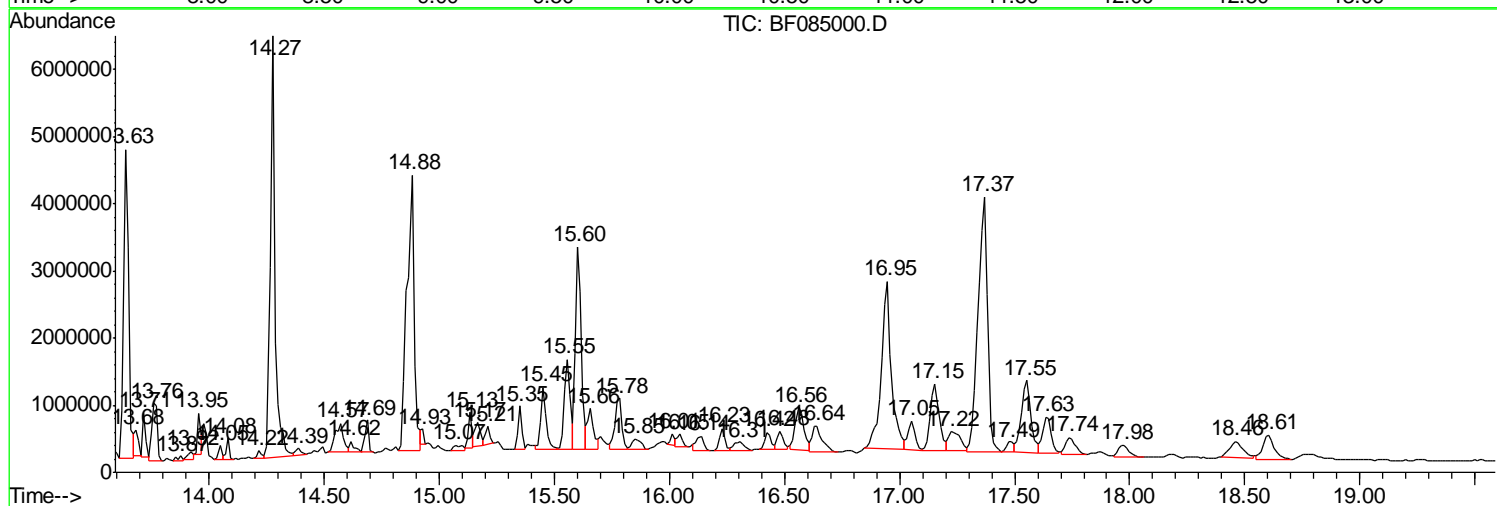
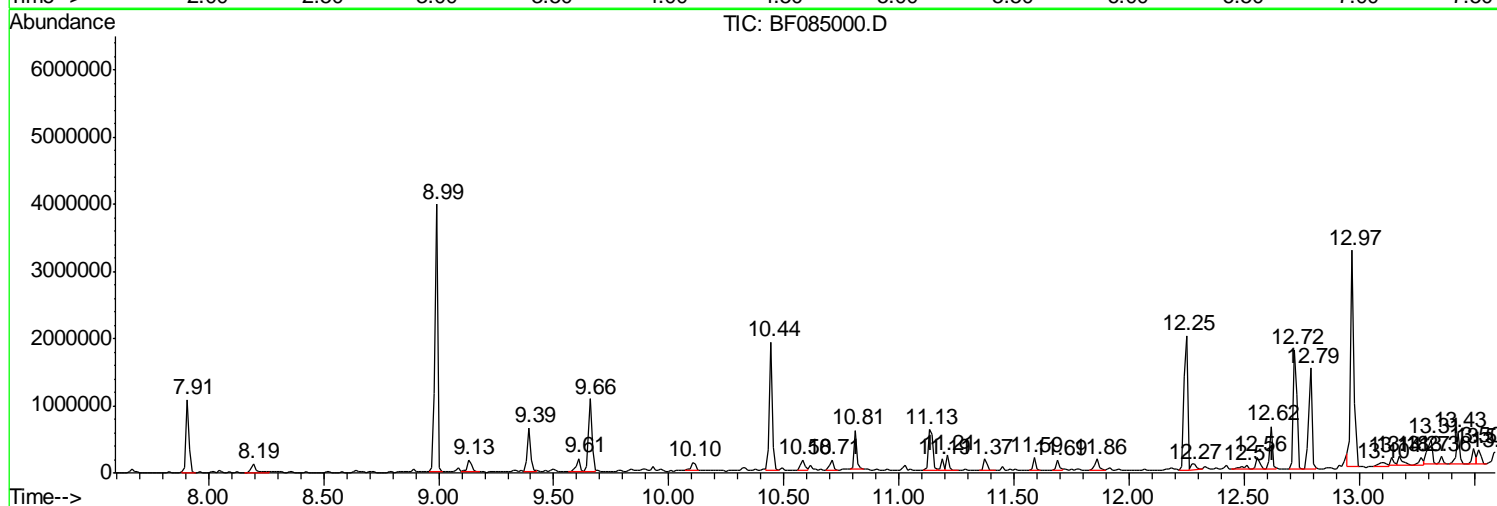
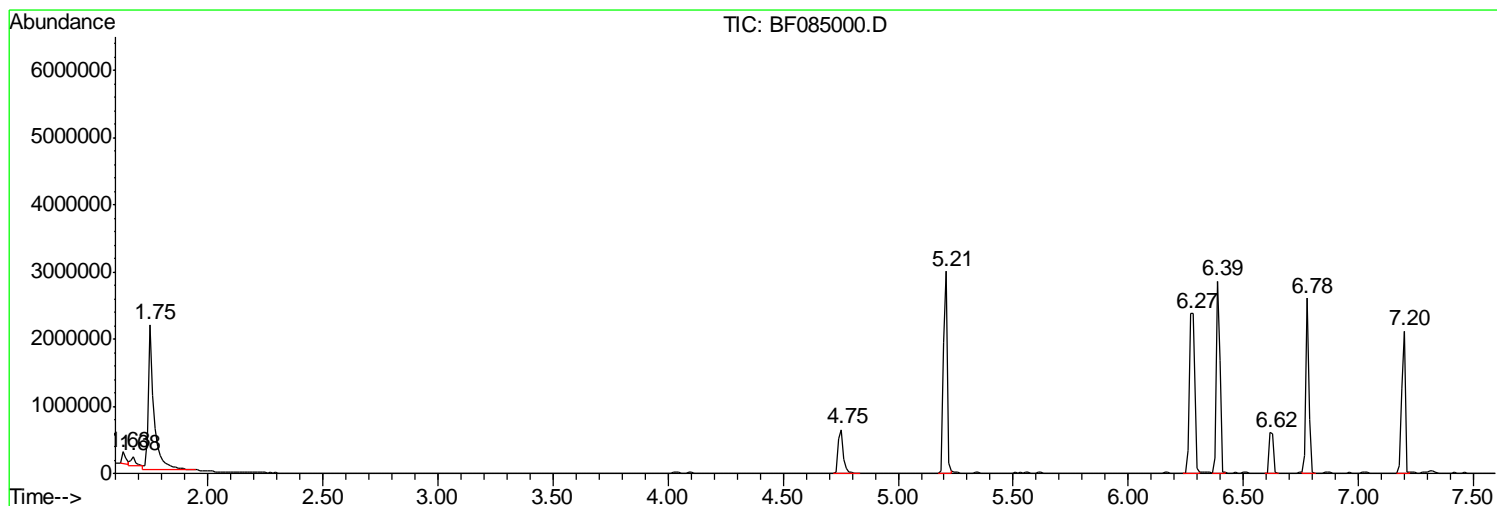
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Instrument :  
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 ClientSampled :  
 S4-B018(22-24)

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF020116.M  
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
 TIC Integration Parameters: LSCINT.P



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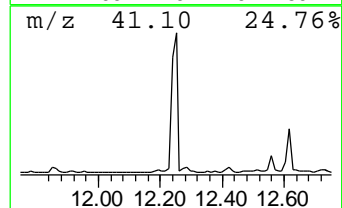
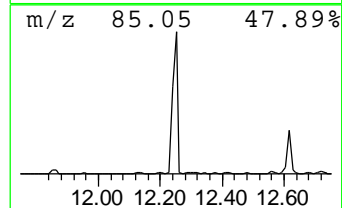
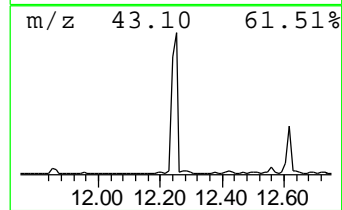
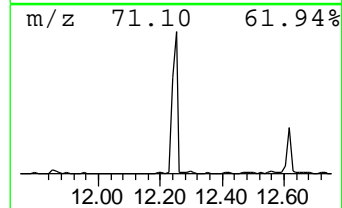
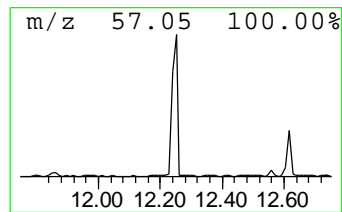
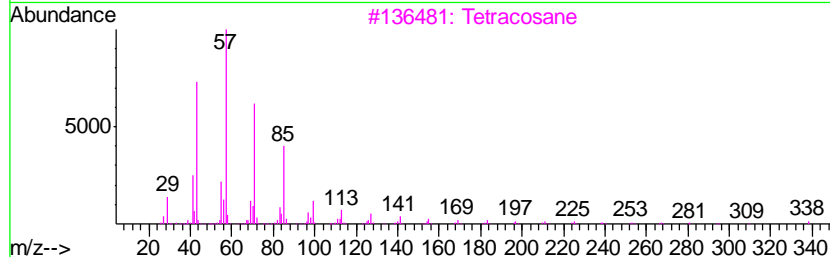
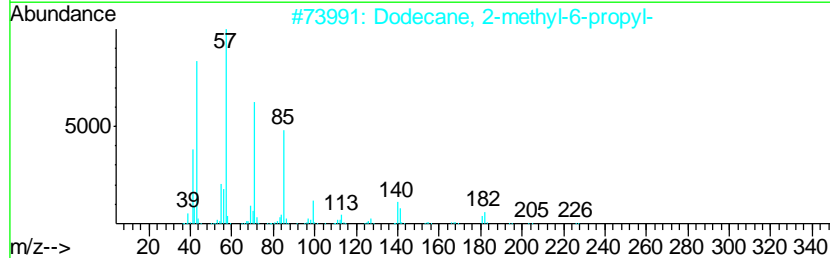
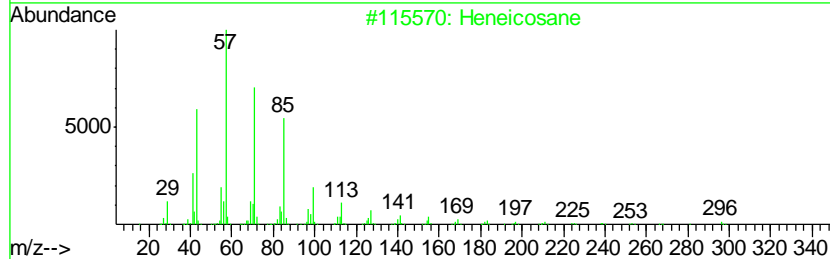
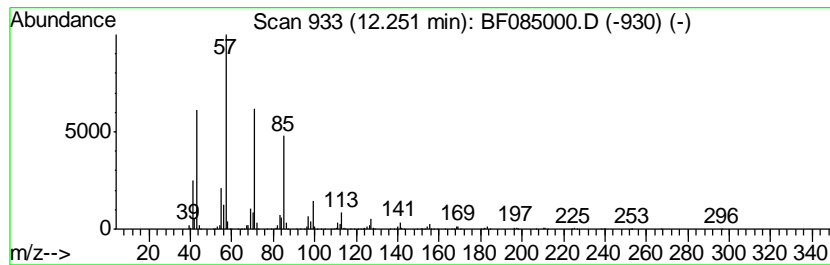
TIC Library : C:\DATABASE\NIST02.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 4 Heneicosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.25	56.49 ng	2360810	Phenanthrene-d10	11.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	98
2		Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	93
3		Tetracosane	338	C24H50	000646-31-1	91
4		Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91
5		Nonadecane	268	C19H40	000629-92-5	91



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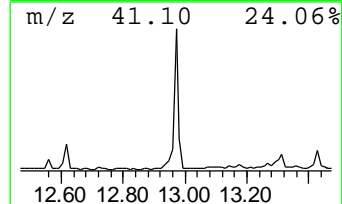
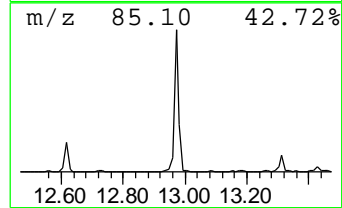
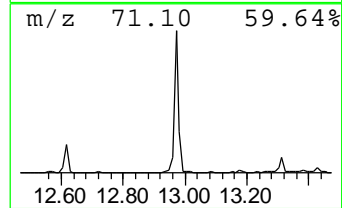
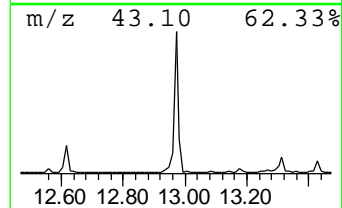
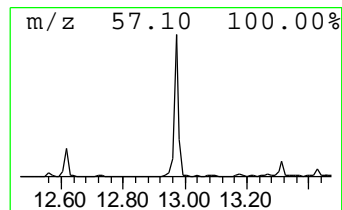
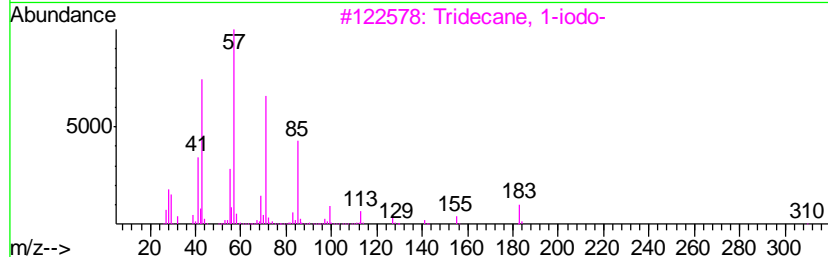
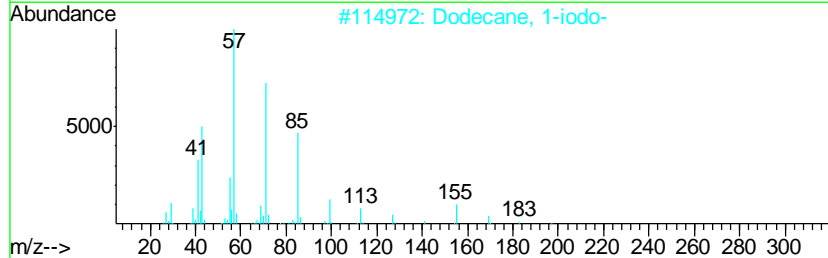
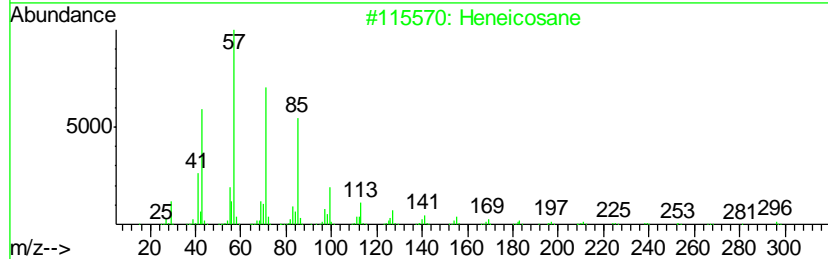
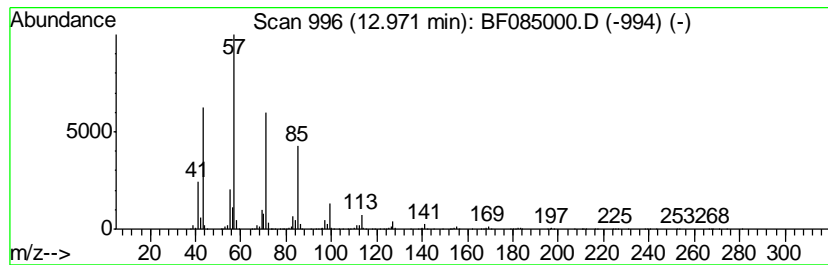
TIC Library : C:\DATABASE\NIST02.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 5 Dodecane, 1-iodo- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.97	43.02 ng	3120470	Chrysene-d12	13.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	90
2		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
3		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86
4		2-Bromo dodecane	248	C12H25Br	013187-99-0	86
5		Heptacosane	380	C27H56	000593-49-7	81



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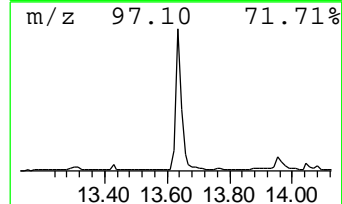
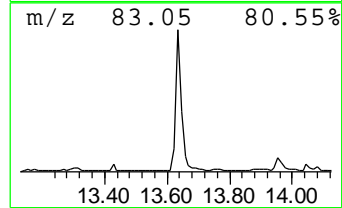
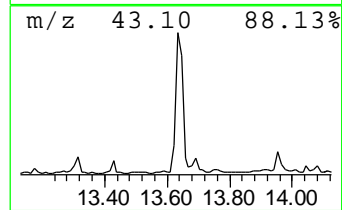
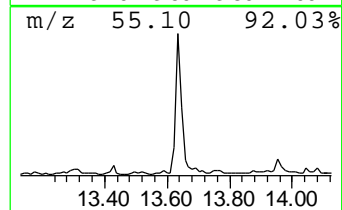
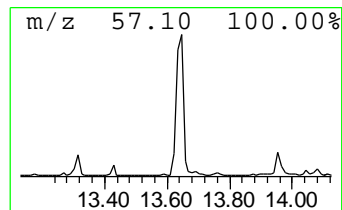
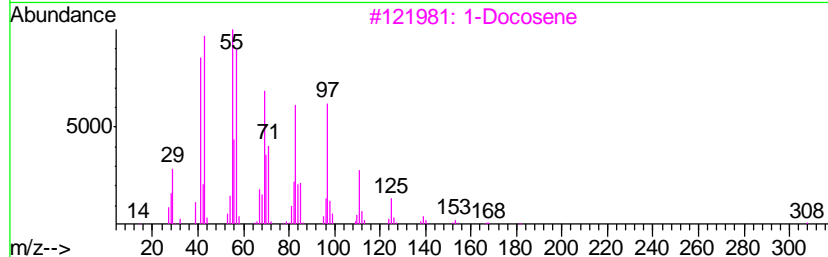
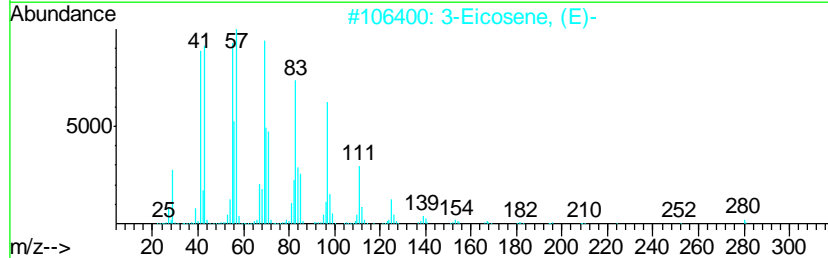
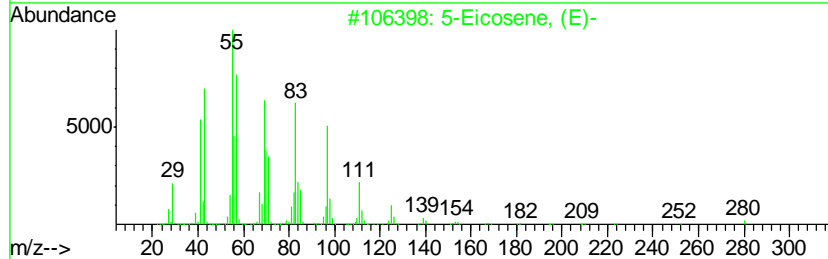
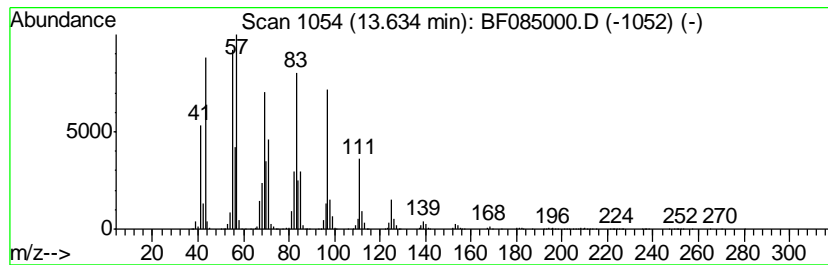
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 TIC Integration Parameters: LSCINT.P

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 Peak Number 6 5-Eicosene, (E)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.63	86.96 ng	6307660	Chrysene-d12	13.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
2		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3		1-Docosene	308	C22H44	001599-67-3	91
4		17-Pentatriacontene	491	C35H70	006971-40-0	91
5		Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	90



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 Operator : SJ/IZ  
 Sample : H1386-06  
 Misc :  
 ALS Vial : 18 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleID :  
 S4-B018(22-24)

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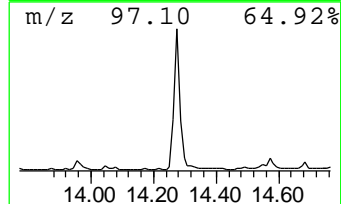
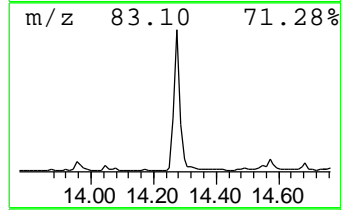
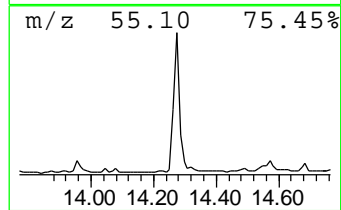
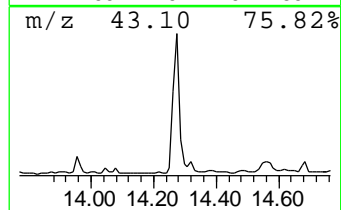
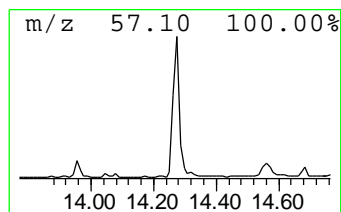
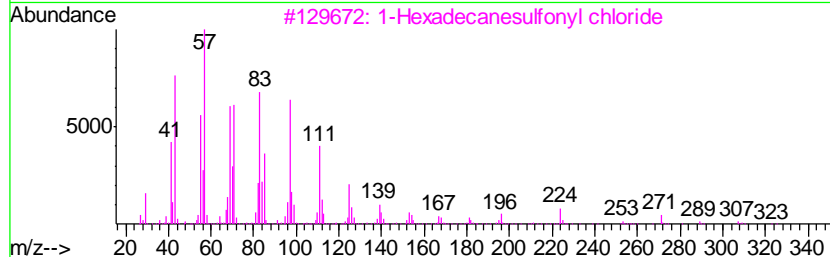
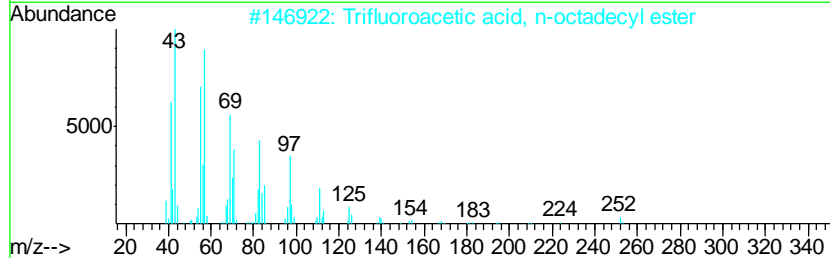
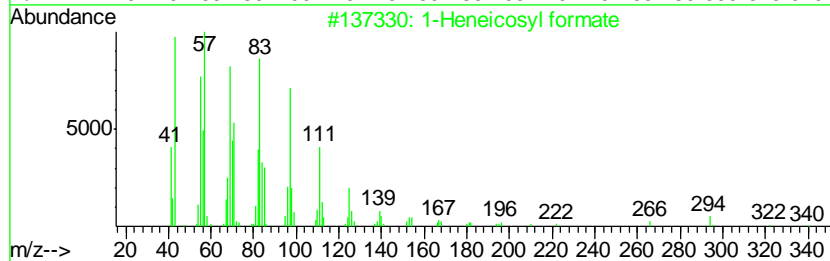
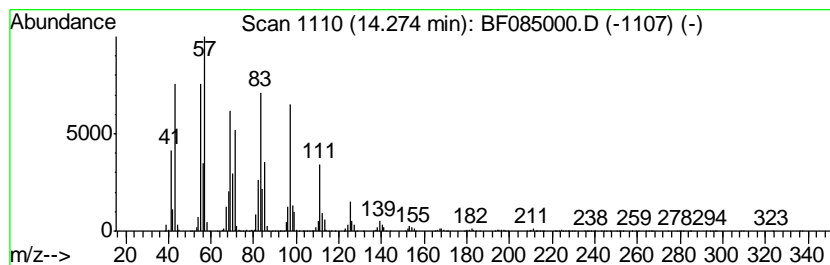
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 Peak Number 7 1-Heneicosyl formate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.27	121.00 ng	8776540	Chrysene-d12	13.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	91
2		Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91
3		1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91
4		1-Docosene	308	C22H44	001599-67-3	90
5		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	90





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 Sample : H1386-06  
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Instrument :  
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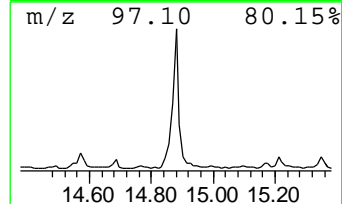
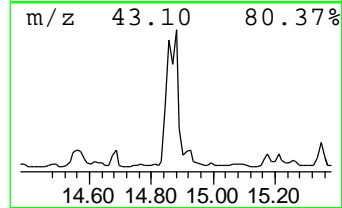
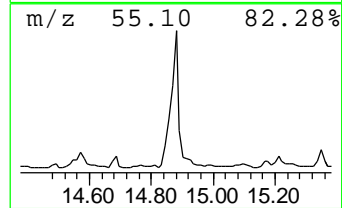
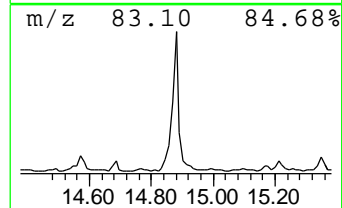
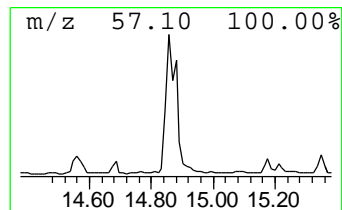
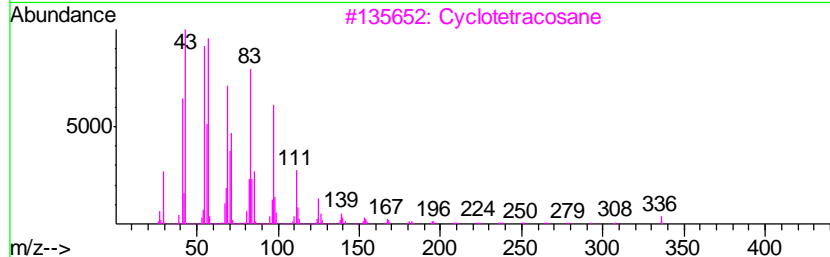
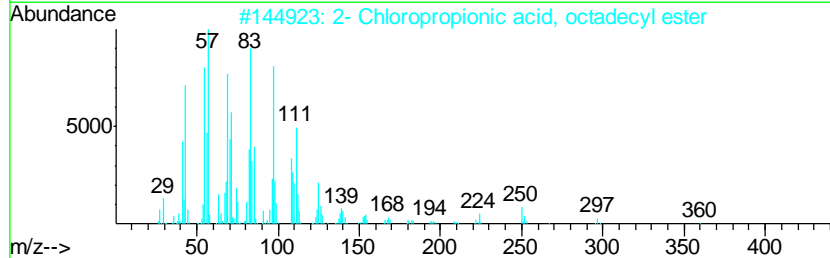
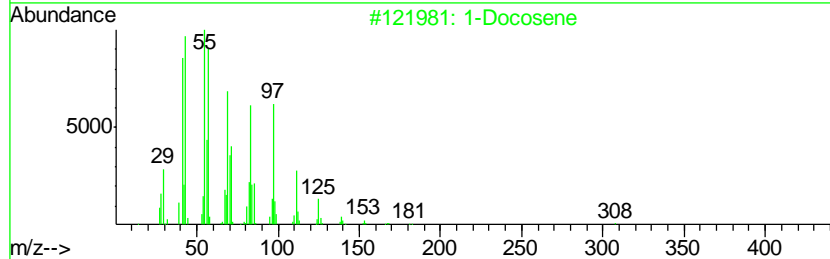
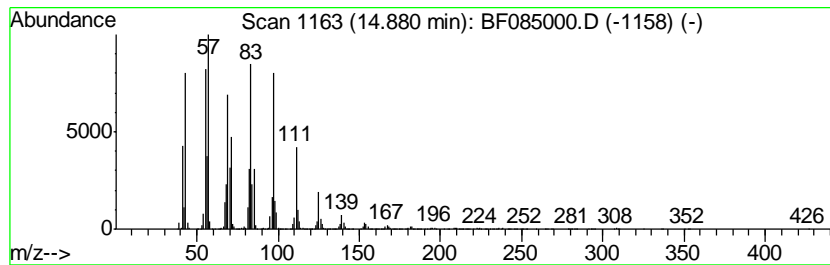
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 TIC Integration Parameters: LSCINT.P

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 Peak Number 8 1-Docosene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.88	287.94 ng	8276730	Perylene-d12	15.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	91
2		2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
3		Cyclotetracosane	336	C24H48	000297-03-0	90
4		1-Heneicosyl formate	340	C22H44O2	077899-03-7	87
5		Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	87



Data Path : Z:\HPCHEM1\BNA F\Data\BF021016\  
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 Operator : SJ/IZ  
 Sample : H1386-06  
 Misc :  
 ALS Vial : 18 Sample Multiplier: 1

Instrument :  
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 ClientSampleID :  
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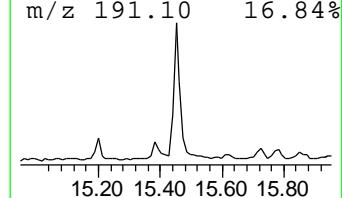
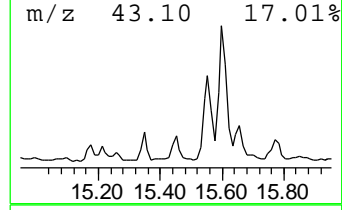
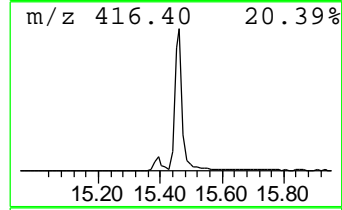
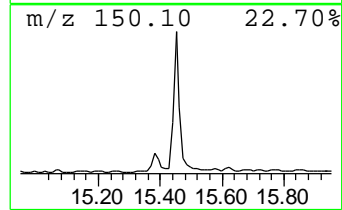
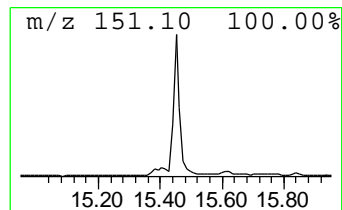
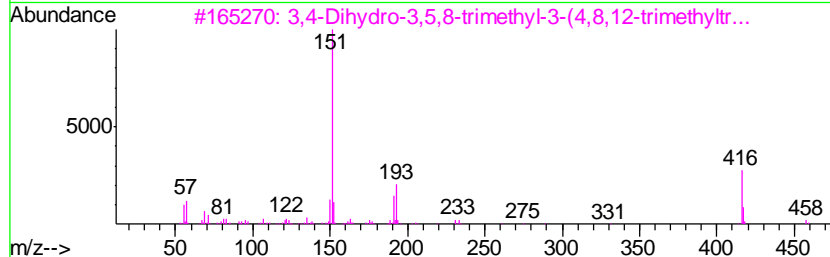
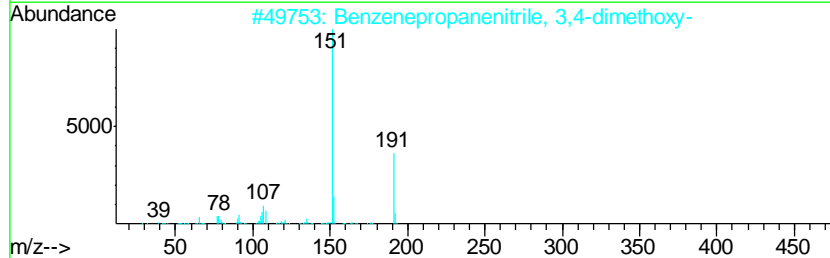
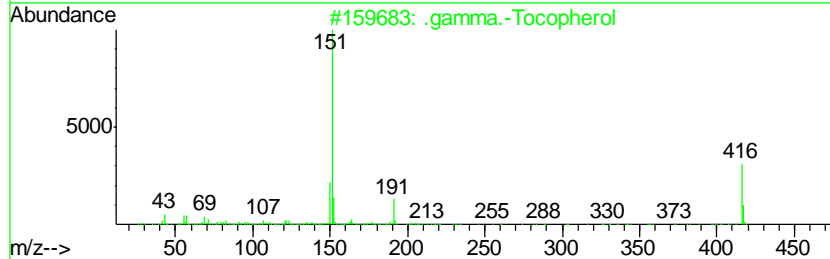
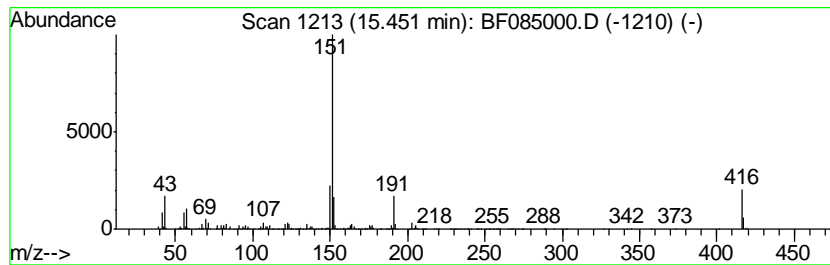
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 TIC Integration Parameters: LSCINT.P

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 Peak Number 9 .gamma.-Tocopherol Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.45	52.00 ng	1494800	Perylene-d12	15.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.gamma.-Tocopherol	416	C28H48O2	007616-22-0	96
2		Benzenepropanenitrile, 3,4-dimet...	191	C11H13NO2	049621-56-9	58
3		3,4-Dihydro-3,5,8-trimethyl-3-(4...	458	C30H50O3	1000105-71-9	43
4		4H-1,3,2-Dioxaborin, 6-ethenyl-2...	208	C12H21BO2	074630-05-0	40
5		p-tert-Octylresorcinol	222	C14H22O2	028122-52-3	38



Data Path : Z:\HPCHEM1\BNA F\Data\BF021016\  
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 Sample : H1386-06  
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Instrument :  
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 ClientSampleID :  
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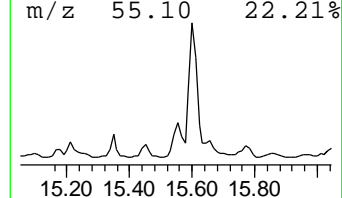
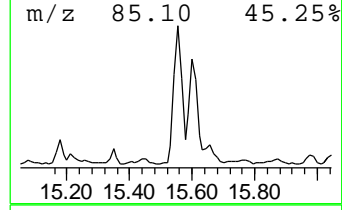
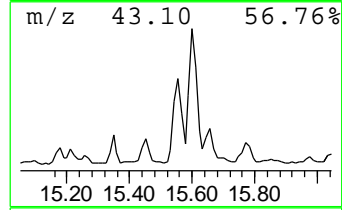
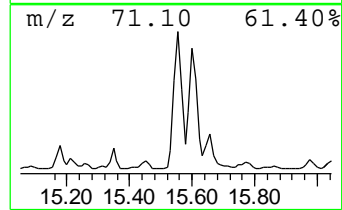
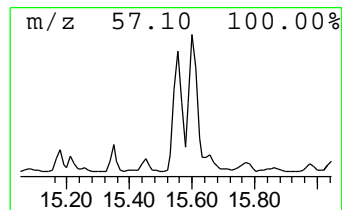
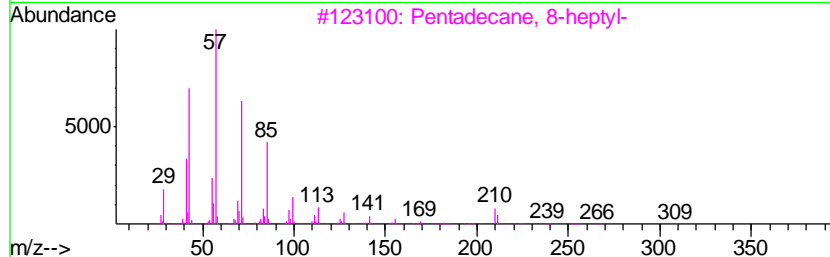
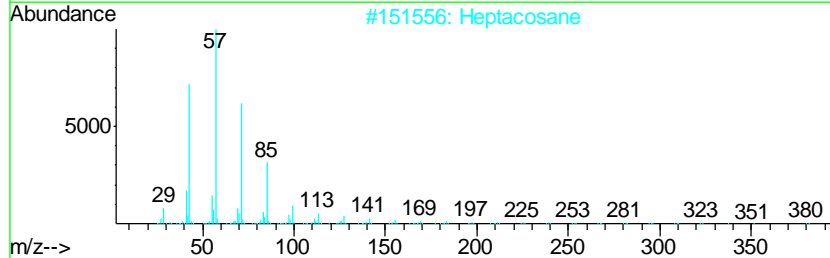
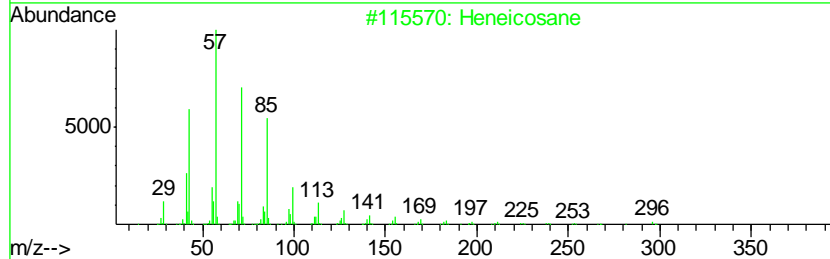
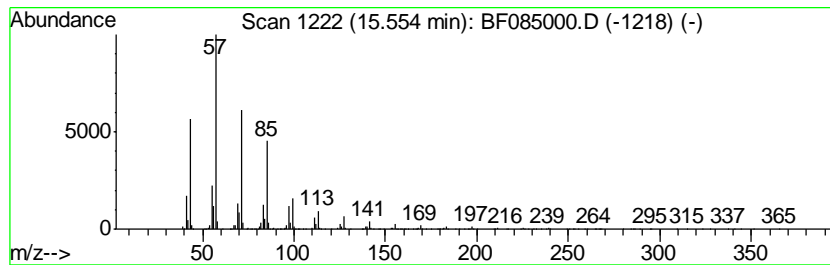
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 TIC Integration Parameters: LSCINT.P

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 Peak Number 10 Heptacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.55	86.33 ng	2481620	Perylene-d12	15.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Heptacosane	380	C27H56	000593-49-7	91
3		Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91
4		Tetracosane	338	C24H50	000646-31-1	90
5		Pentacosane	352	C25H52	000629-99-2	90



Data Path : Z:\HPCHEM1\BNA F\Data\BF021016\  
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 Operator : SJ/IZ  
 Sample : H1386-06  
 Misc :  
 ALS Vial : 18 Sample Multiplier: 1

Instrument :  
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 ClientSampleID :  
 S4-B018(22-24)

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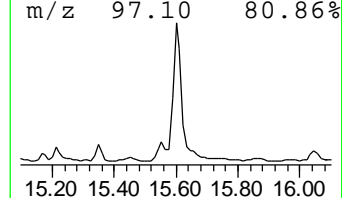
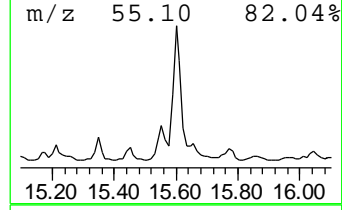
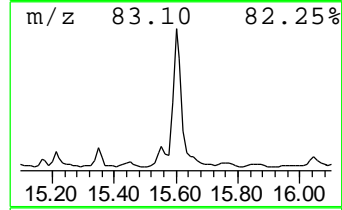
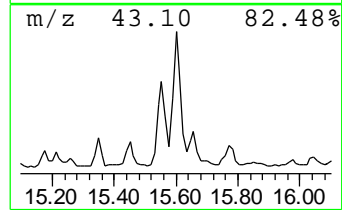
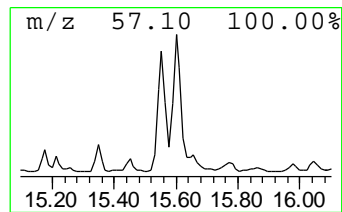
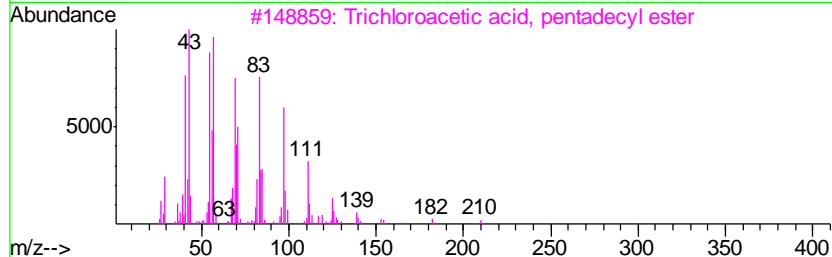
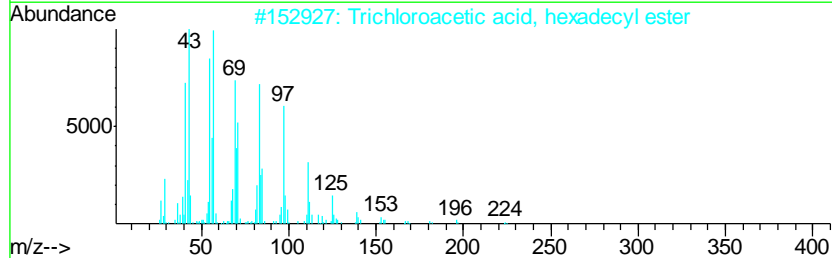
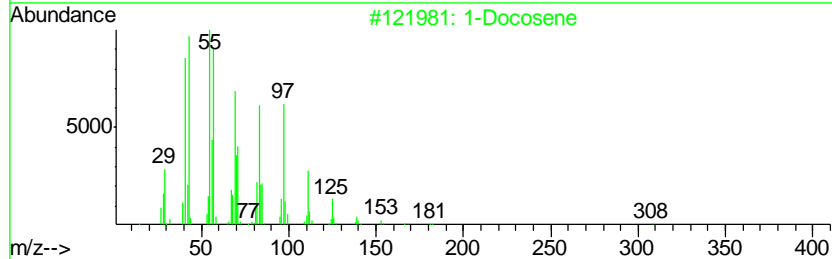
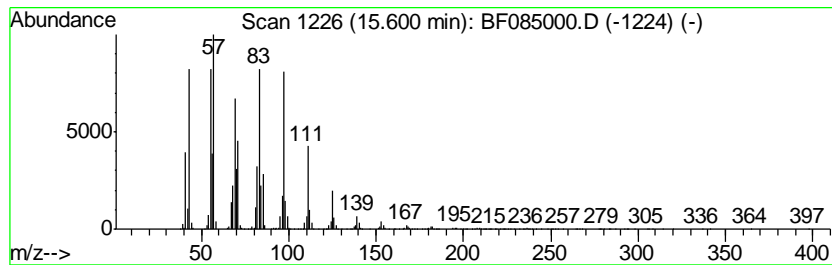
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 TIC Integration Parameters: LSCINT.P

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 Peak Number 11 Trichloroacetic acid, penta... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.60	188.81 ng	5427210	Perylene-d12	15.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	91
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	81
3		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	74
4		1-Nonadecene	266	C19H38	018435-45-5	72
5		11-Tricosene	322	C23H46	052078-56-5	72



Data Path : Z:\HPCHEM1\BNA F\Data\BF021016\  
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 Acq On : 10 Feb 2016 18:36  
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 Sample : H1386-06  
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Instrument :  
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 ClientSampleID :  
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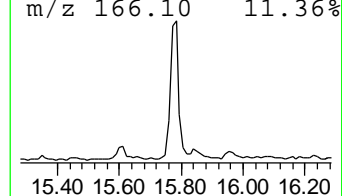
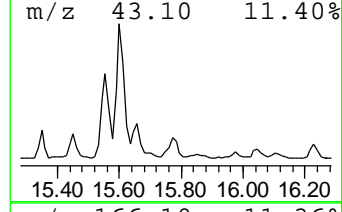
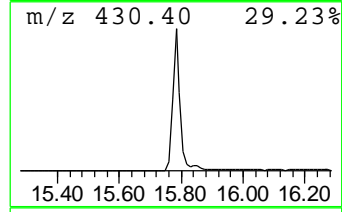
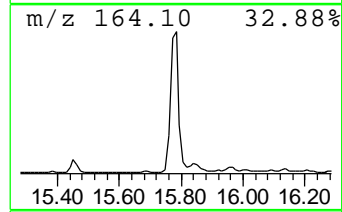
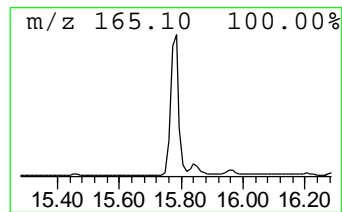
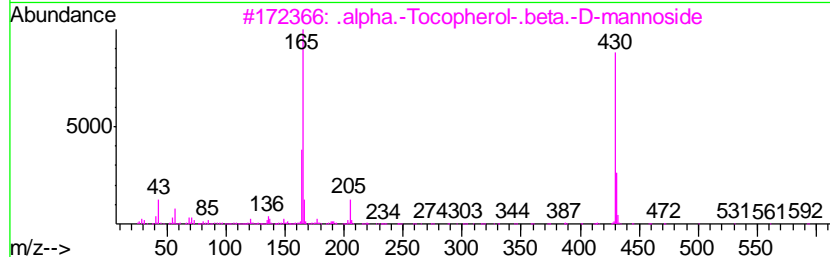
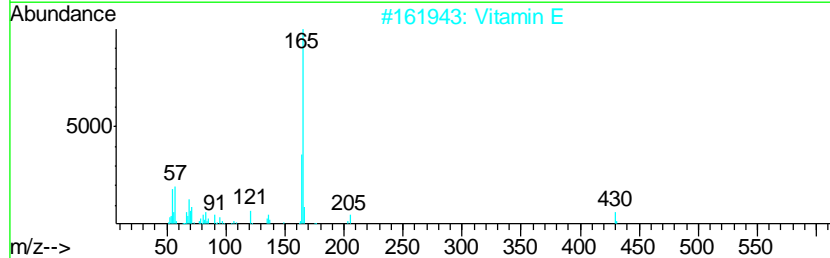
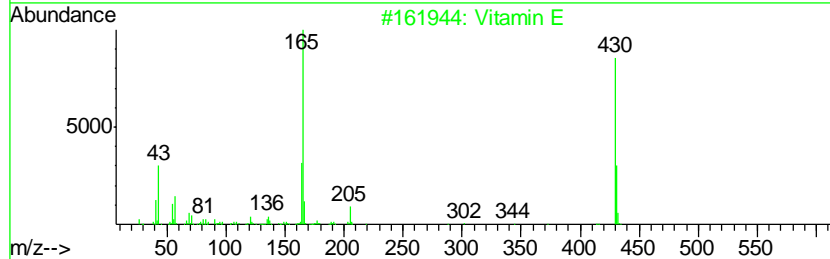
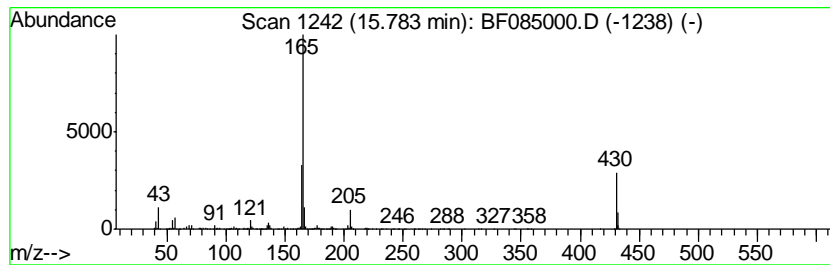
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 TIC Integration Parameters: LSCINT.P

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 Peak Number 12 Vitamin E Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.78	55.76 ng	1602760	Perylene-d12	15.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Vitamin E	430	C29H50O2	010191-41-0	95
2		Vitamin E	430	C29H50O2	000059-02-9	94
3		.alpha.-Tocopherol-.beta.-D-mann...	592	C35H60O7	1000156-68-2	64
4		4-Amino-3-methoxy-pyrazolo[3,4-d]...	165	C6H7N5O	111375-22-5	53
5		Propanenitrile, 3-[methyl(4-nitr...	205	C10H11N3O2	097473-81-9	40



Data Path : Z:\HPCHEM1\BNA F\Data\BF021016\  
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 Acq On : 10 Feb 2016 18:36  
 Operator : SJ/IZ  
 Sample : H1386-06  
 Misc :  
 ALS Vial : 18 Sample Multiplier: 1

Instrument :  
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 ClientSampled :  
 S4-B018(22-24)

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF020116.M  
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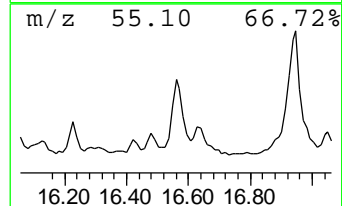
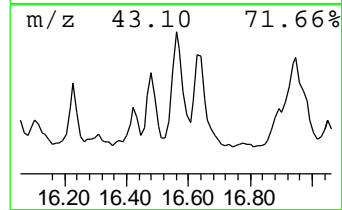
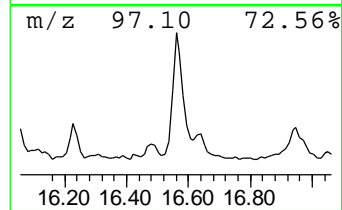
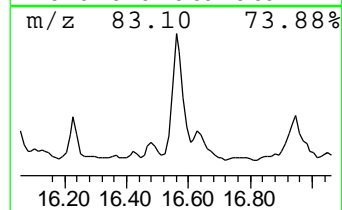
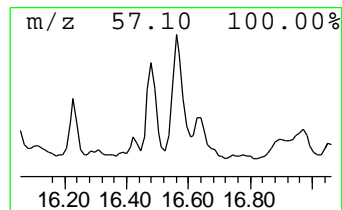
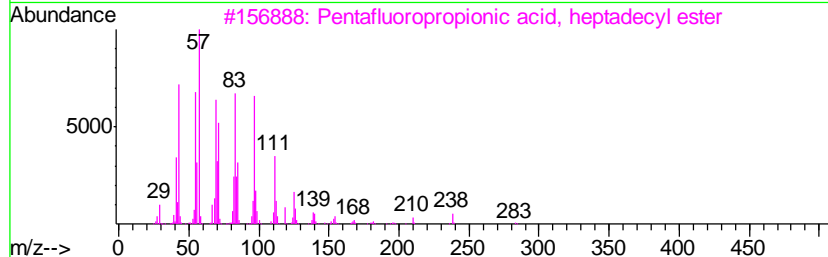
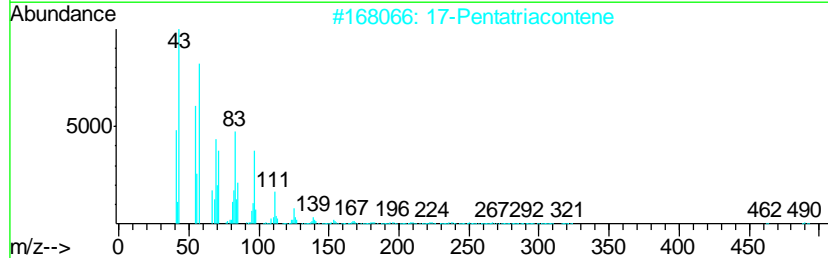
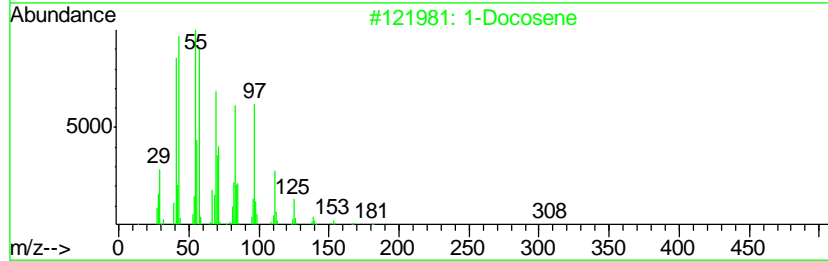
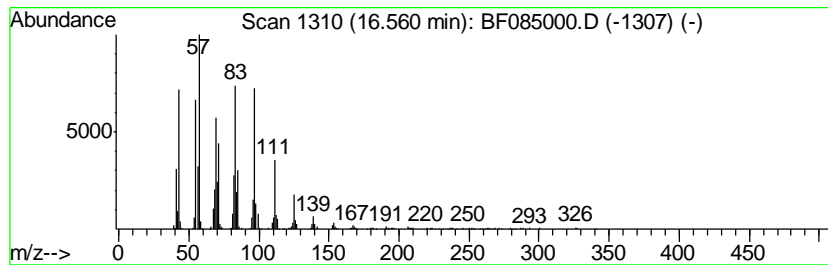
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 TIC Integration Parameters: LSCINT.P

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 Peak Number 13 17-Pentatriacontene Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.56	54.80 ng	1575270	Perylene-d12	15.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	91
2		17-Pentatriacontene	491	C35H70	006971-40-0	91
3		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	91
4		1-Tricosene	322	C23H46	018835-32-0	90
5		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	86



Data Path : Z:\HPCHEM1\BNA F\Data\BF021016\  
 Data File : BF085000.D  
 Acq On : 10 Feb 2016 18:36  
 Operator : SJ/IZ  
 Sample : H1386-06  
 Misc :  
 ALS Vial : 18 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleID :  
 S4-B018(22-24)

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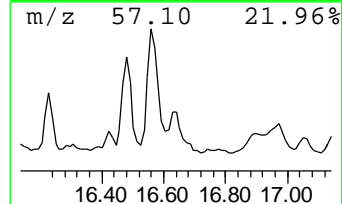
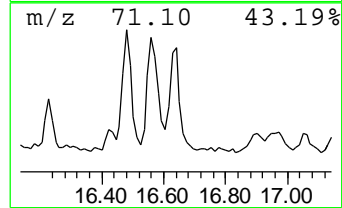
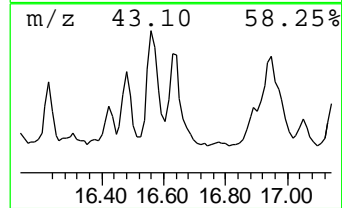
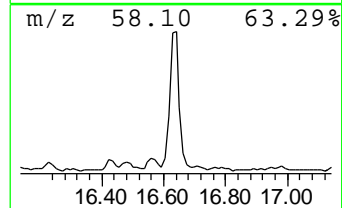
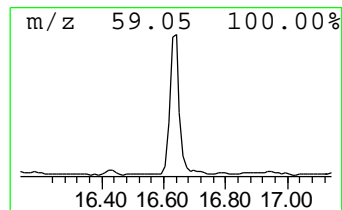
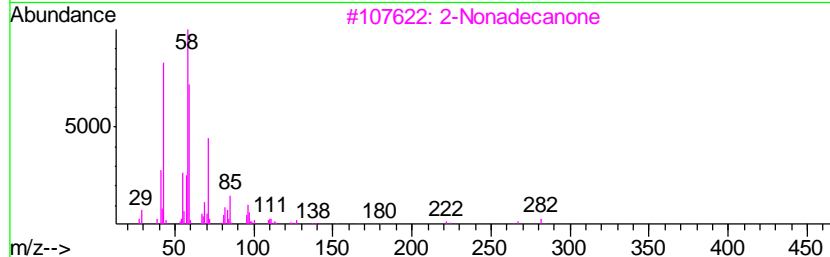
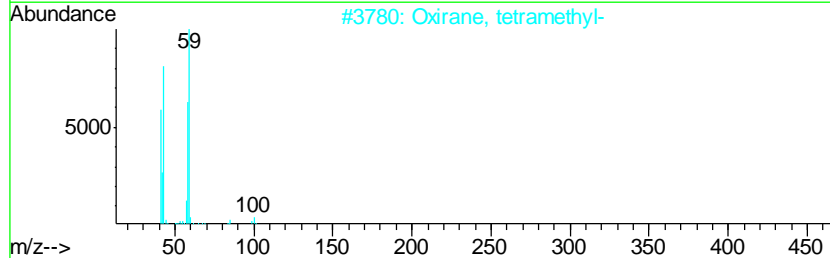
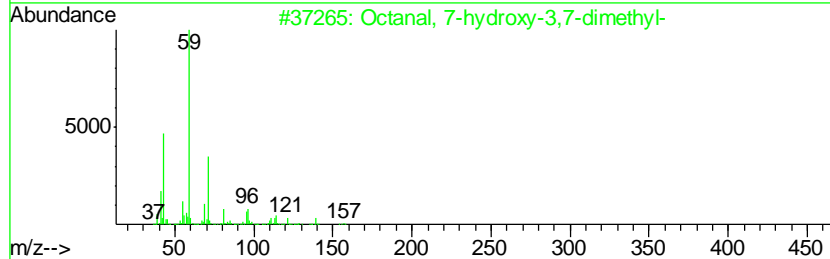
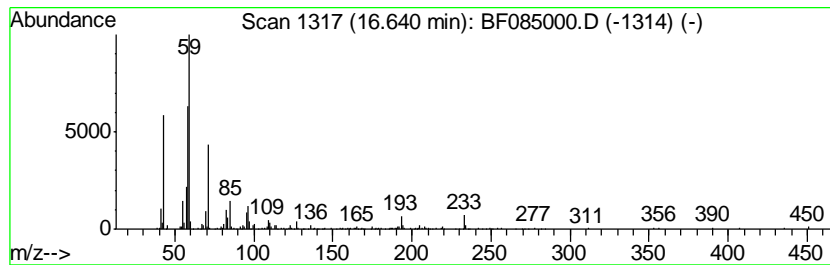
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 TIC Integration Parameters: LSCINT.P

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 Peak Number 14 Octanal, 7-hydroxy-3,7-dime... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.64	40.40 ng	1161370	Perylene-d12	15.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octanal, 7-hydroxy-3,7-dimethyl-	172	C10H20O2	000107-75-5	50
2		Oxirane, tetramethyl-	100	C6H12O	005076-20-0	49
3		2-Nonadecanone	282	C19H38O	000629-66-3	38
4		2-Nonanone	142	C9H18O	000821-55-6	38
5		2-Hexadecanone	240	C16H32O	018787-63-8	37



Data Path : Z:\HPCHEM1\BNA F\Data\BF021016\  
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 Operator : SJ/IZ  
 Sample : H1386-06  
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 ALS Vial : 18 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleID :  
 S4-B018(22-24)

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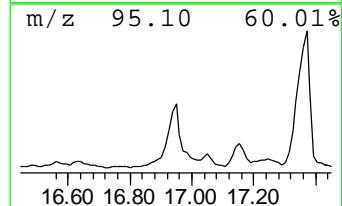
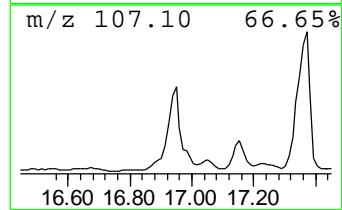
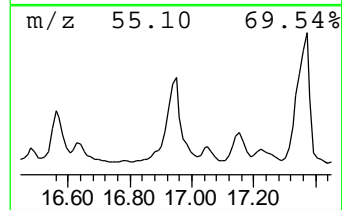
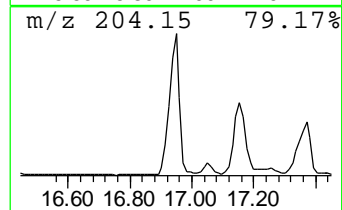
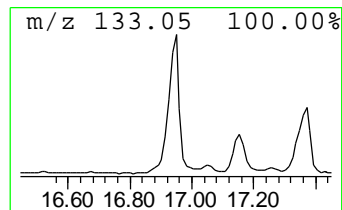
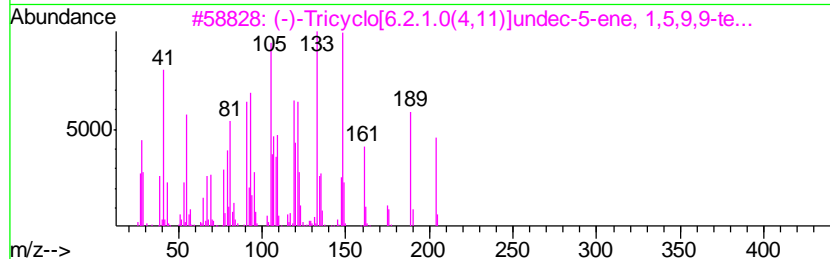
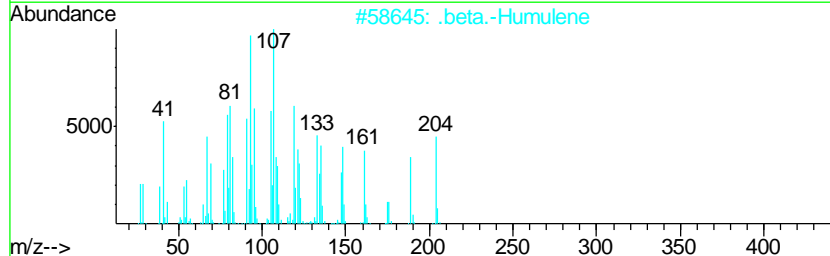
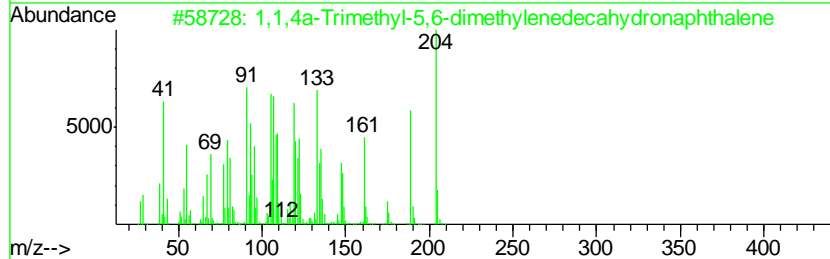
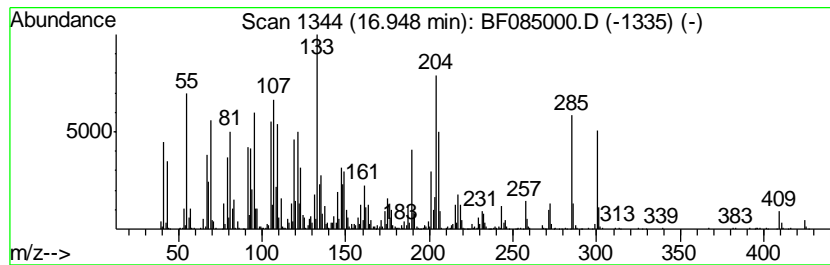
TIC Library : C:\DATABASE\NIST02.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 15 unknown16.95 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.95	260.40 ng	7485210	Perylene-d12	15.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	49
2		.beta.-Humulene	204	C15H24	000116-04-1	45
3		(-)-Tricyclo[6.2.1.0(4,11)]undec...	204	C15H24	1000154-06-7	45
4		Lup-20(29)-en-3-one	424	C30H48O	001617-70-5	42
5		1,4-Methano-1H-indene, octahydro...	204	C15H24	087064-18-4	41





Data Path : Z:\HPCHEM1\BNA F\Data\BF021016\  
 Data File : BF085000.D  
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 Operator : SJ/IZ  
 Sample : H1386-06  
 Misc :  
 ALS Vial : 18 Sample Multiplier: 1

Instrument :  
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 ClientSampleID :  
 S4-B018(22-24)

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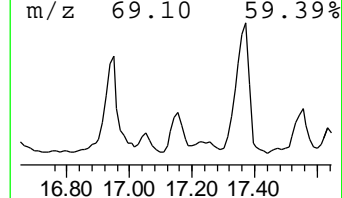
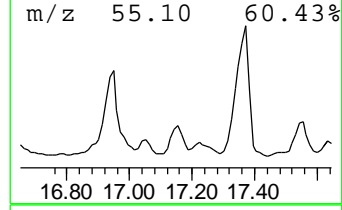
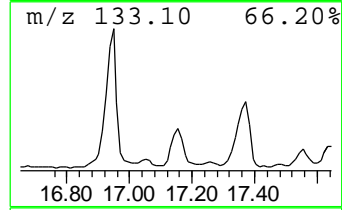
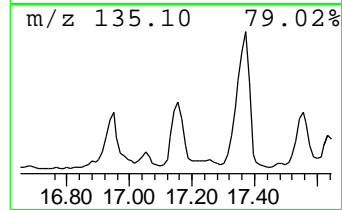
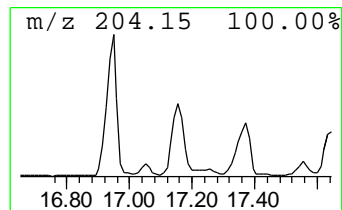
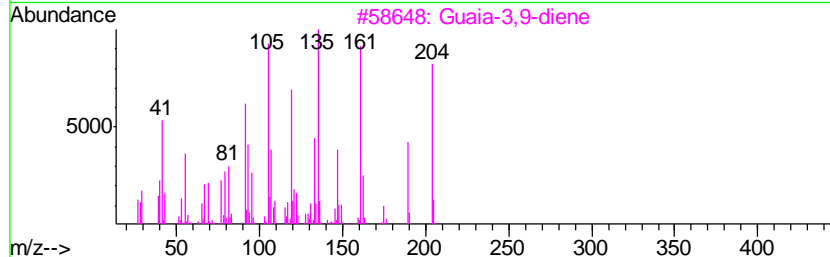
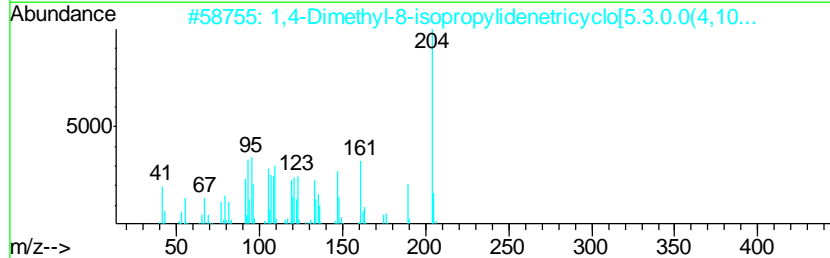
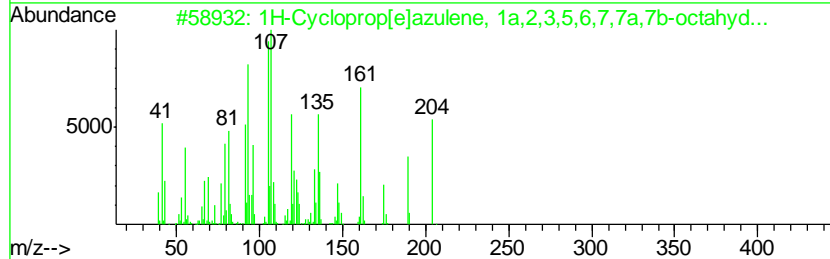
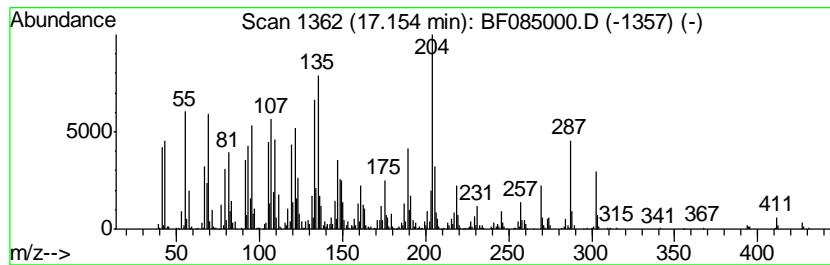
TIC Library : C:\DATABASE\NIST02.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 16 1H-Cycloprop[el]azulene, 1a,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.15	89.52 ng	2573310	Perylene-d12	15.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Cycloprop[el]azulene, 1a,2,3,5...	204	C15H24	021747-46-6	50
2		1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1000140-07-7	50
3		Guaia-3,9-diene	204	C15H24	000489-83-8	50
4		2,5,5,8a-Tetramethyl-6,7,8,8a-te...	204	C14H20O	124957-09-1	46
5		1H-3a,7-Methanoazulene, 2,3,6,7,...	204	C15H24	000560-32-7	43



Data Path : Z:\HPCHEM1\BNA F\Data\BF021016\  
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 Sample : H1386-06  
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Instrument :  
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 ClientSampleID :  
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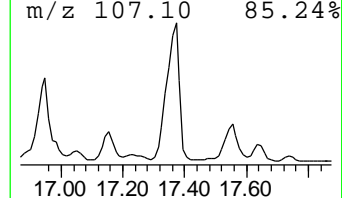
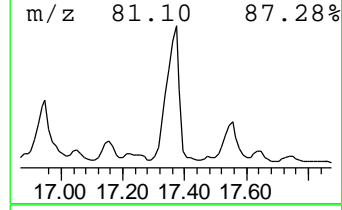
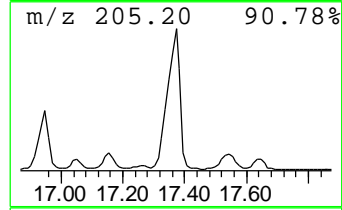
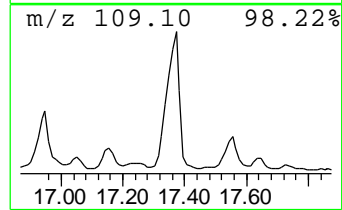
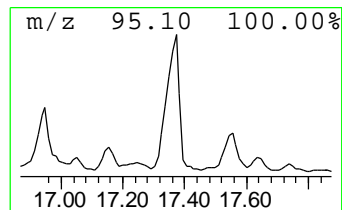
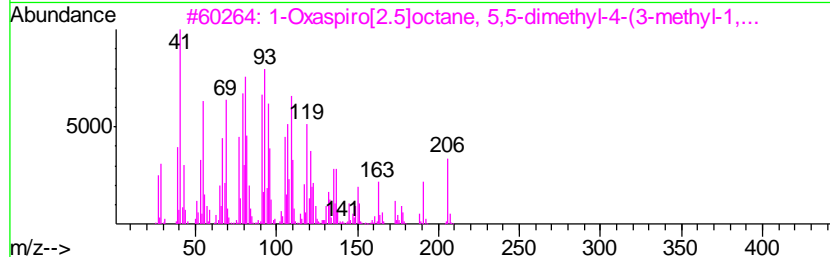
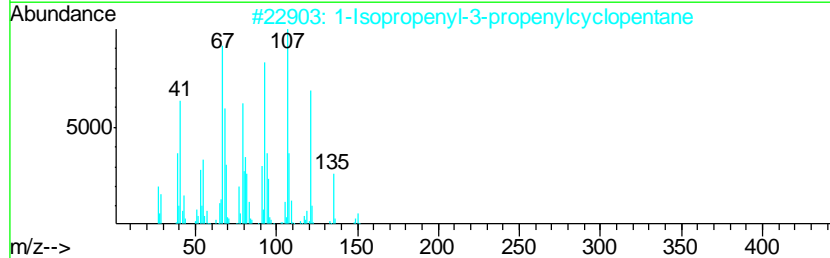
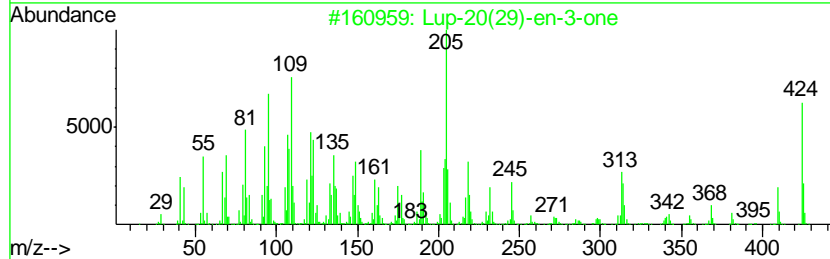
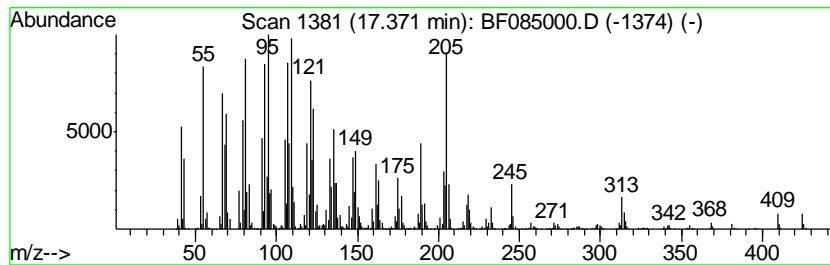
TIC Library : C:\DATABASE\NIST02.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 17 Lup-20(29)-en-3-one Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.37	375.30 ng	10787800	Perylene-d12	15.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Lup-20(29)-en-3-one	424	C30H48O	001617-70-5	60
2		1-Isopropenyl-3-propenylcyclopent...	150	C11H18	1000192-81-2	58
3		1-Oxaspiro[2.5]octane, 5,5-dimet...	206	C14H22O	1000195-92-1	45
4		1,5-Cyclododecadiene, 1,5-dimethyl...	204	C15H24	015423-57-1	44
5		Eudesma-4(14),11-diene	204	C15H24	1000152-04-3	43



Data Path : Z:\HPCHEM1\BNA F\Data\BF021016\  
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 Operator : SJ/IZ  
 Sample : H1386-06  
 Misc :  
 ALS Vial : 18 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleID :  
 S4-B018(22-24)

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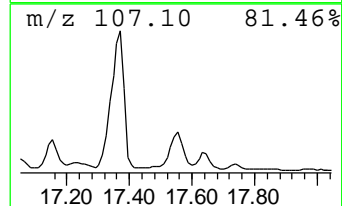
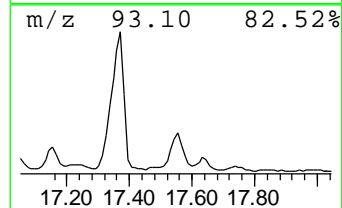
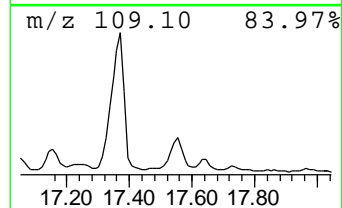
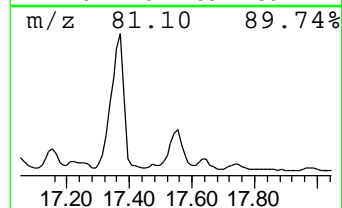
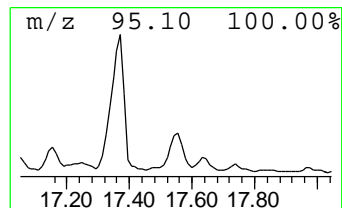
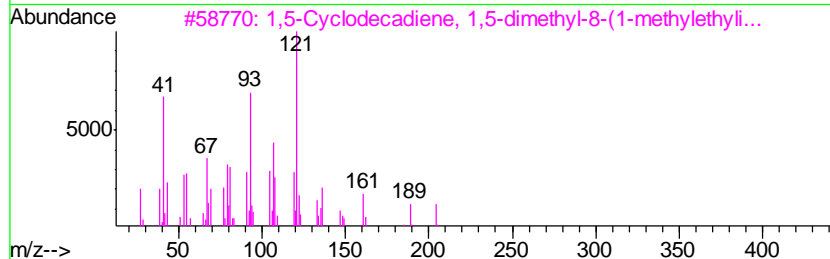
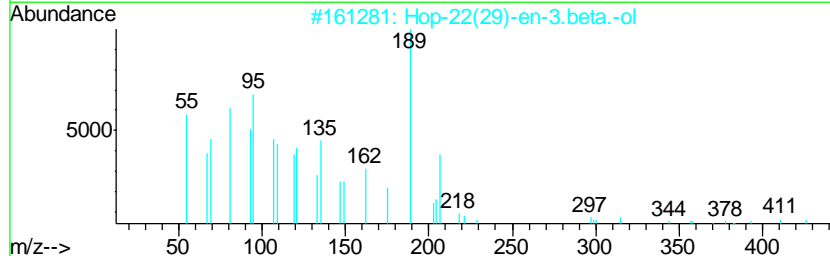
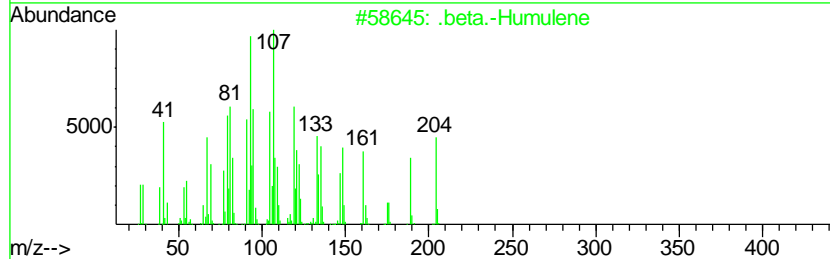
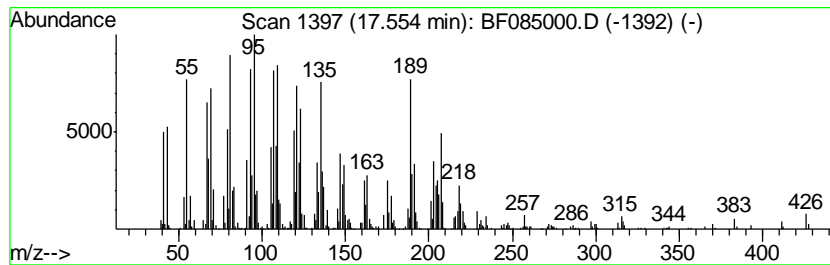
TIC Library : C:\DATABASE\NIST02.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 18 .beta.-Humulene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.55	109.72 ng	3153860	Perylene-d12	15.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.beta.-Humulene	204	C15H24	000116-04-1	78
2		Hop-22(29)-en-3.beta.-ol	426	C30H50O	058801-23-3	78
3		1,5-Cyclodecadiene, 1,5-dimethyl...	204	C15H24	015423-57-1	46
4		1R,4S,7S,11R-2,2,4,8-Tetramethyl...	204	C15H24	1000140-07-6	43
5		Longifolenaldehyde	220	C15H24O	019890-84-7	41



Data Path : Z:\HPCHEM1\BNA F\Data\BF021016\  
 Data File : BF085000.D  
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 Sample : H1386-06  
 Misc :  
 ALS Vial : 18 Sample Multiplier: 1

Instrument :  
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 ClientSampleID :  
 S4-B018(22-24)

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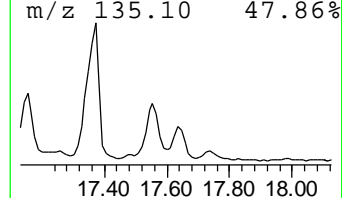
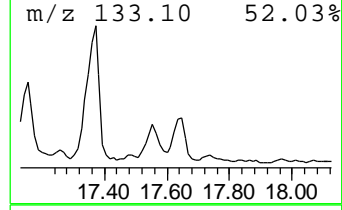
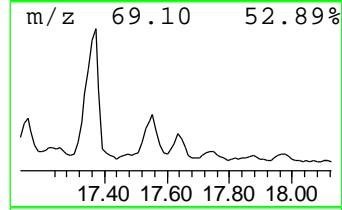
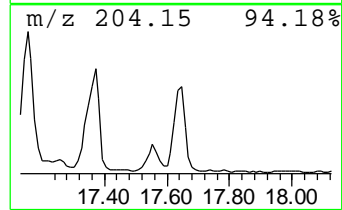
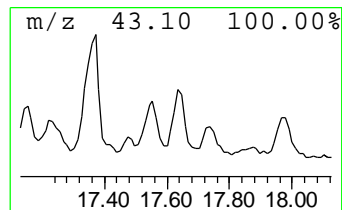
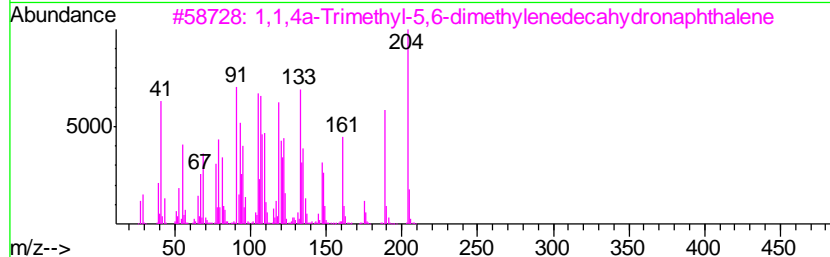
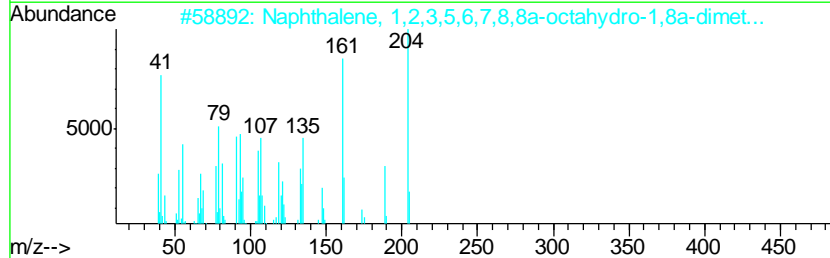
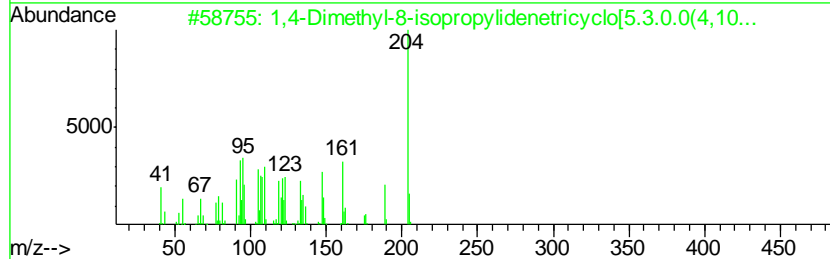
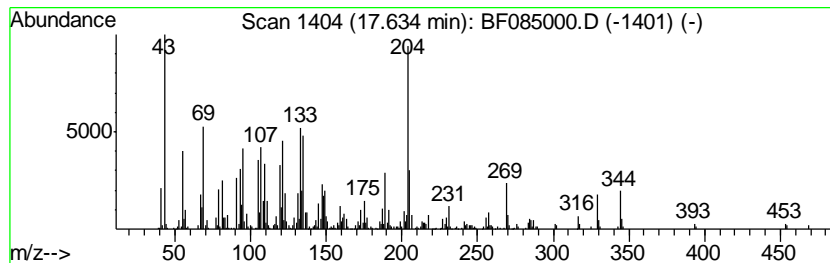
TIC Library : C:\DATABASE\NIST02.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 19 1,4-Dimethyl-8-isopropylide... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.63	49.11 ng	1411530	Perylene-d12	15.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1000140-07-7	64
2		Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	58
3		1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	50
4		3H-3a,7-Methanoazulene, 2,4,5,6,...	204	C15H24	002387-78-2	18
5		1,4-Naphthalenedione, 5,8-dihydr...	204	C11H8O4	014554-09-7	14



Data Path : Z:\HPCHEM1\BNA F\Data\BF021016\  
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 Misc :  
 ALS Vial : 18 Sample Multiplier: 1

Instrument :  
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 ClientSampled :  
 S4-B018(22-24)

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF020116.M  
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

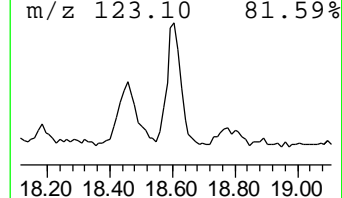
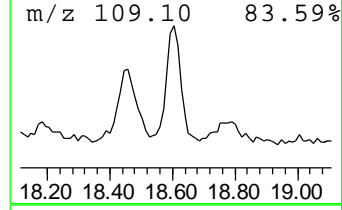
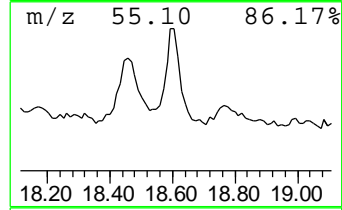
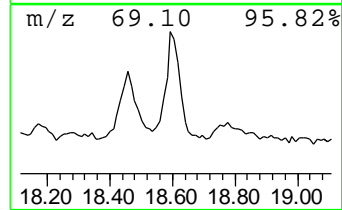
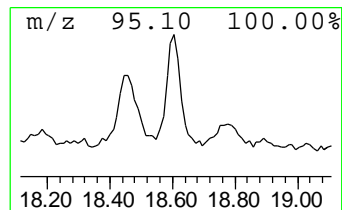
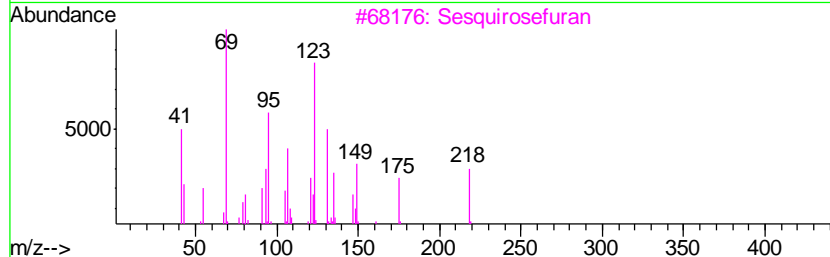
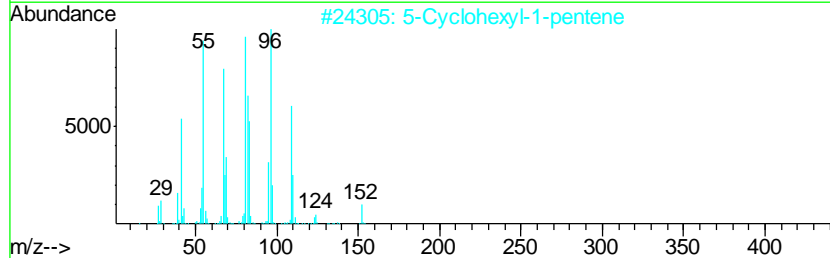
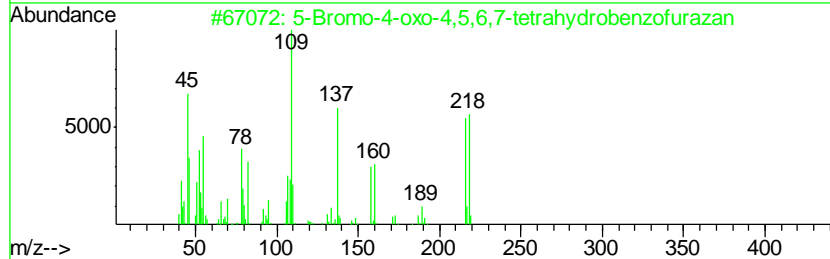
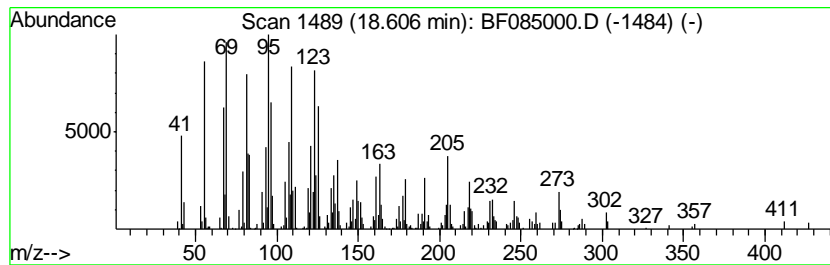
TIC Library : C:\DATABASE\NIST02.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 20 5-Bromo-4-oxo-4,5,6,7-tetra... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.61	41.05 ng	1179890	Perylene-d12	15.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	59
2		5-Cyclohexyl-1-pentene	152	C11H20	005729-54-4	44
3		Sesquirosefuran	218	C15H22O	039007-93-7	41
4		3-Cyclopentylpropionic acid, 3-c...	216	C11H17ClO2	1000292-47-2	38
5		1-Formyl-2,2,6-trimethyl-3-(3-me...	220	C15H24O	108287-18-9	38



Data Path : Z:\HPCHEM1\BNA\_F\Data\BF021016\  
 Data File : BF085000.D  
 Acq On : 10 Feb 2016 18:36  
 Operator : SJ/IZ  
 Sample : H1386-06  
 Misc :  
 ALS Vial : 18 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 S4-B018(22-24)

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF020116.M  
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Heneicosane	12.25	56.5	ng	2360810	4	11.14	835870	20.0
Dodecane, 1-iodo-	12.97	43.0	ng	3120470	5	13.77	1450690	20.0
5-Eicosene, (E)-	13.63	87.0	ng	6307660	5	13.77	1450690	20.0
1-Heneicosyl formate	14.27	121.0	ng	8776540	5	13.77	1450690	20.0
1-Docosene	14.88	287.9	ng	8276730	6	15.13	574894	20.0
.gamma.-Tocopherol	15.45	52.0	ng	1494800	6	15.13	574894	20.0
Heptacosane	15.55	86.3	ng	2481620	6	15.13	574894	20.0
Trichloroacetic a...	15.60	188.8	ng	5427210	6	15.13	574894	20.0
Vitamin E	15.78	55.8	ng	1602760	6	15.13	574894	20.0
17-Pentatriacontene	16.56	54.8	ng	1575270	6	15.13	574894	20.0
Octanal, 7-hydrox...	16.64	40.4	ng	1161370	6	15.13	574894	20.0
unknown16.95	16.95	260.4	ng	7485210	6	15.13	574894	20.0
1H-Cycloprop[e]az...	17.15	89.5	ng	2573310	6	15.13	574894	20.0
Lup-20(29)-en-3-one	17.37	375.3	ng	10787800	6	15.13	574894	20.0
.beta.-Humulene	17.55	109.7	ng	3153860	6	15.13	574894	20.0
1,4-Dimethyl-8-is...	17.63	49.1	ng	1411530	6	15.13	574894	20.0
5-Bromo-4-oxo-4,5...	18.61	41.0	ng	1179890	6	15.13	574894	20.0