

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072717\  
 Data File : BF097136.D  
 Acq On : 27 Jul 2017 21:37  
 Operator : SJ/JU  
 Sample : I4422-13  
 Misc :  
 ALS Vial : 43 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 72-11940-COMP

Integration Parameters: rteint.p  
 Integrator: RTE  
 Smoothing : ON Filtering: 5  
 Sampling : 1 Min Area: 3 % of largest Peak  
 Start Thrs: 0.2 Max Peaks: 100  
 Stop Thrs : 0 Peak Location: TOP

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

Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF072517.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	4.628	462	466	478	rBV	150342	241204	9.13%	1.086%
2	5.087	539	544	564	rBV	2232304	2457177	93.02%	11.063%
3	6.151	720	725	739	rBV	2552231	2641453	100.00%	11.892%
4	6.257	739	743	747	rBV	2398342	2375341	89.93%	10.694%
5	6.486	778	782	793	rVB	781577	671482	25.42%	3.023%
6	6.639	804	808	819	rBV	1836379	1754068	66.41%	7.897%
7	7.057	874	879	882	rBV	1478624	1534807	58.10%	6.910%
8	7.769	996	1000	1005	rBV	1143948	949288	35.94%	4.274%
9	8.851	1178	1184	1187	rBV	2259042	2301666	87.14%	10.363%
10	9.245	1247	1251	1254	rBV	344716	269748	10.21%	1.214%
11	9.516	1292	1297	1300	rBV	930154	845263	32.00%	3.806%
12	9.969	1371	1374	1377	rVB	41884	32128	1.22%	0.145%
13	10.186	1406	1411	1414	rBV2	22613	29251	1.11%	0.132%
14	10.298	1426	1430	1437	rBV	1280467	1281798	48.53%	5.771%
15	10.451	1450	1456	1461	rBV2	62274	106430	4.03%	0.479%
16	10.886	1526	1530	1532	rBV	35125	34328	1.30%	0.155%
17	10.916	1532	1535	1538	rVB	61607	58910	2.23%	0.265%
18	10.986	1543	1547	1551	rBV	945348	784645	29.71%	3.533%
19	11.063	1556	1560	1568	rVB6	14137	29163	1.10%	0.131%
20	11.545	1639	1642	1644	rBV	85020	77515	2.93%	0.349%
21	12.192	1749	1752	1756	rVB	41712	36219	1.37%	0.163%
22	12.321	1770	1774	1781	rBV2	32906	41667	1.58%	0.188%
23	12.415	1786	1790	1795	rVB	48350	45647	1.73%	0.206%
24	12.574	1812	1817	1820	rBV	1827836	1844296	69.82%	8.303%
25	13.480	1967	1971	1981	rBV3	106598	143110	5.42%	0.644%
26	13.610	1988	1993	1996	rBV	667793	631043	23.89%	2.841%
27	14.598	2159	2161	2163	rBV	31408	32533	1.23%	0.146%
28	14.774	2189	2191	2196	rBV6	17966	29745	1.13%	0.134%
29	14.904	2211	2213	2218	rVB	36878	45867	1.74%	0.207%
30	14.956	2218	2222	2226	rBV	477076	532272	20.15%	2.396%
31	15.074	2239	2242	2248	rBV8	24085	49627	1.88%	0.223%
32	15.256	2272	2273	2280	rBV6	25690	37937	1.44%	0.171%
33	15.598	2329	2331	2336	rBV5	19836	32534	1.23%	0.146%
34	15.768	2359	2360	2367	rVB4	24016	34146	1.29%	0.154%

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Smoothing : ON Filtering: 5  
Sampling : 1 Min Area: 3 % of largest Peak  
Start Thrs: 0.2 Max Peaks: 100  
Stop Thrs : 0 Peak Location: TOP

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

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35	15.886	2374	2380	2388	rBV4	29581	95714	3.62%	0.431%
36	16.180	2425	2430	2435	rBV2	21290	45071	1.71%	0.203%
37	18.309	2789	2792	2796	rBV6	17537	30713	1.16%	0.138%
38	19.003	2906	2910	2913	rBV5	17876	27653	1.05%	0.124%

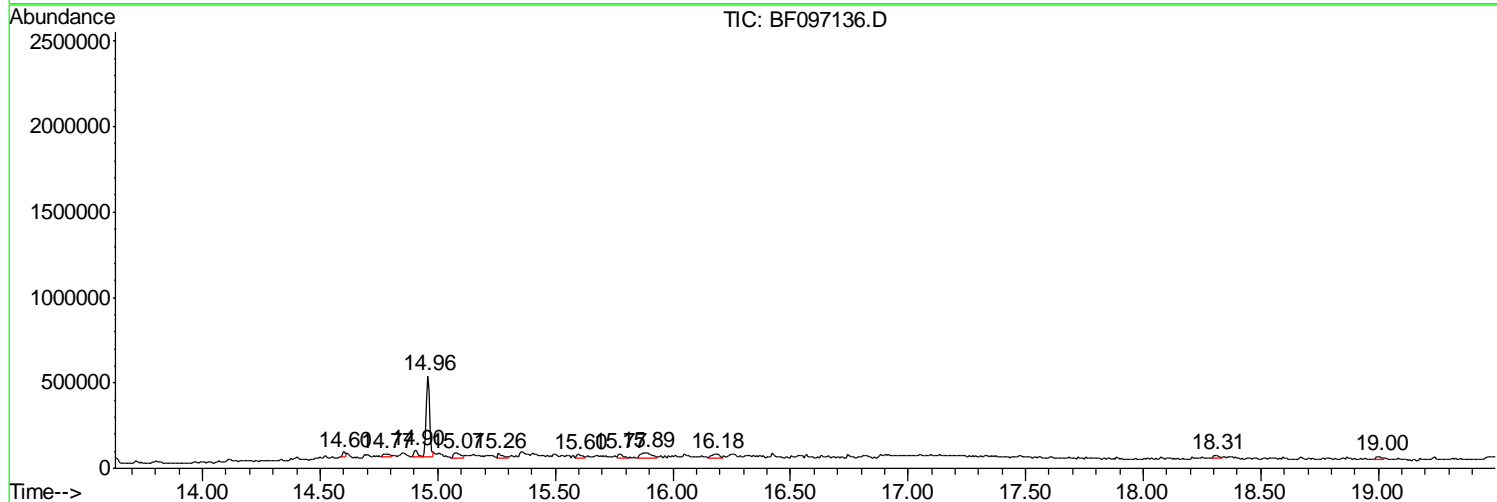
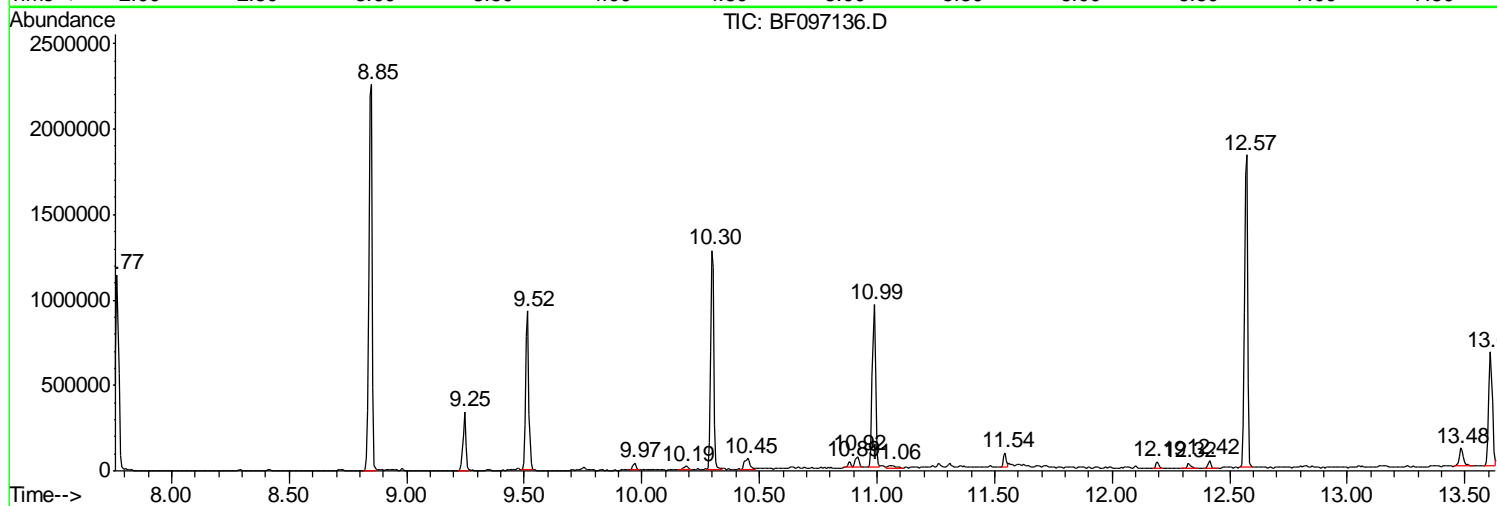
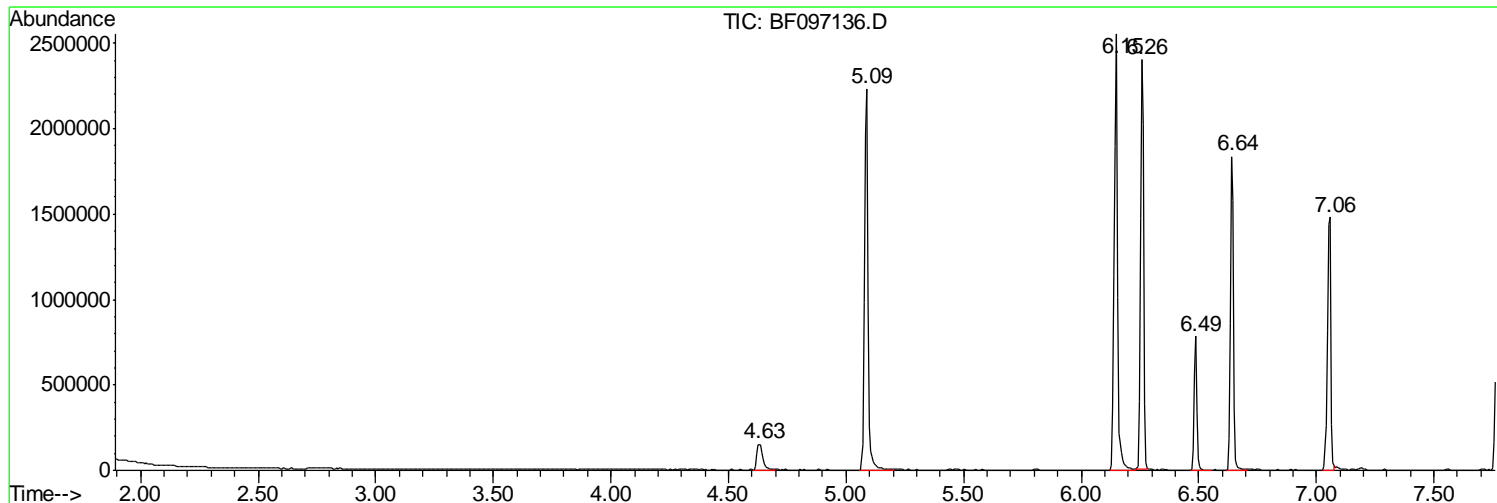
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF072517.M  
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TIC Library : C:\DATABASE\NIST11.L  
 TIC Integration Parameters: LSCINT.P



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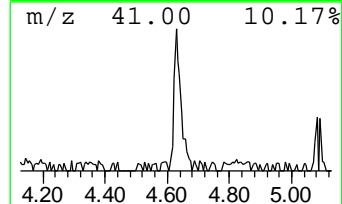
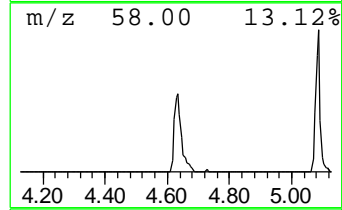
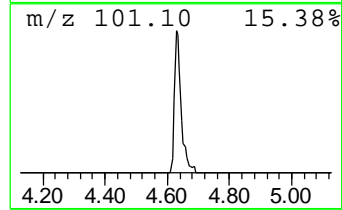
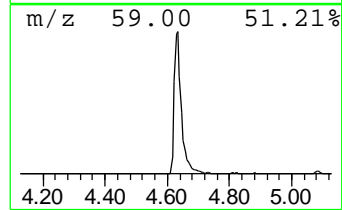
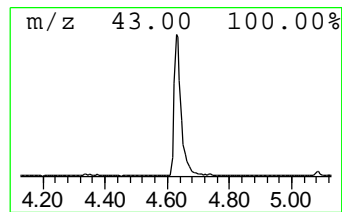
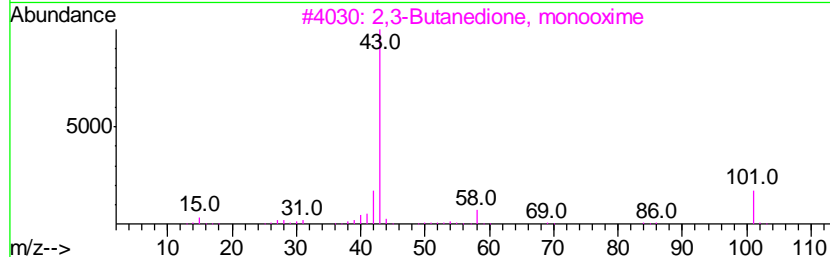
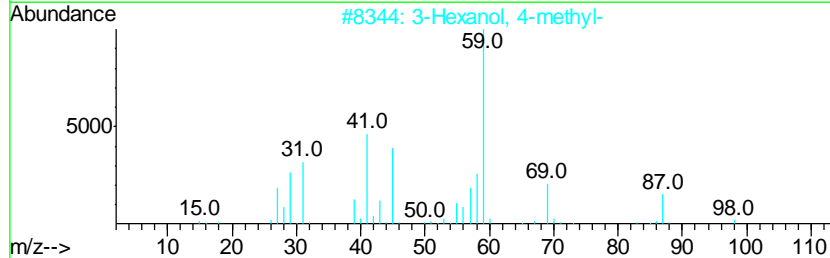
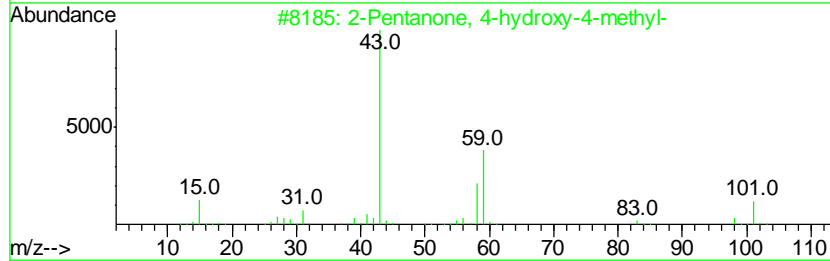
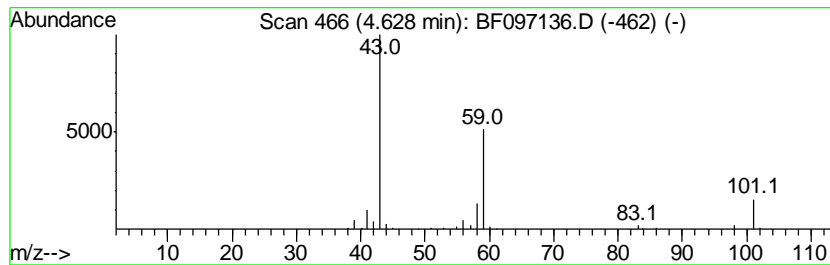
TIC Library : C:\DATABASE\NIST11.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.63	7.18 ng	241204	1,4-Dichlorobenzene-d4	6.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	40
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5		5-Oxohexanenitrile	111	C6H9NO	010412-98-3	9



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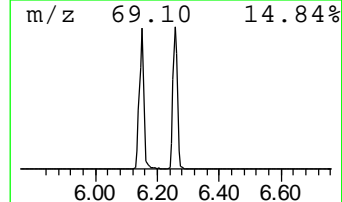
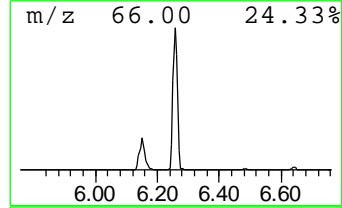
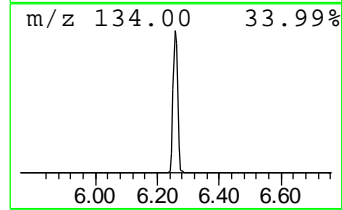
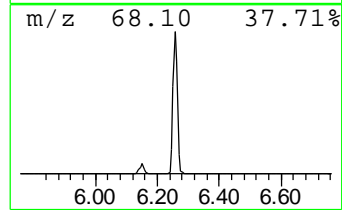
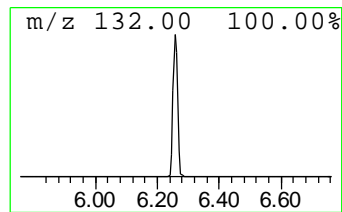
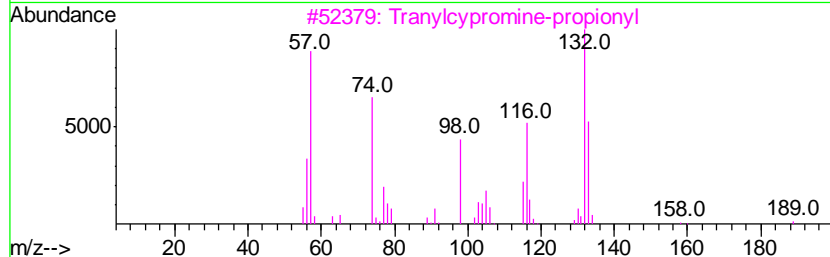
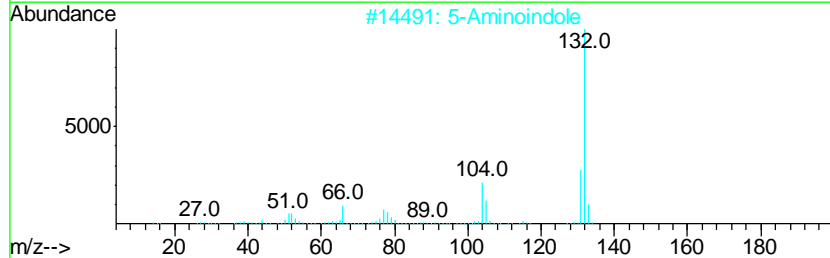
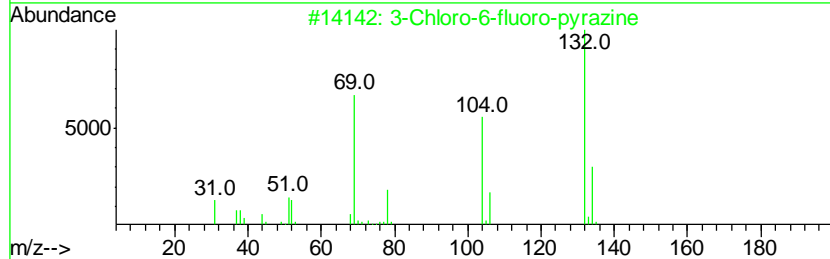
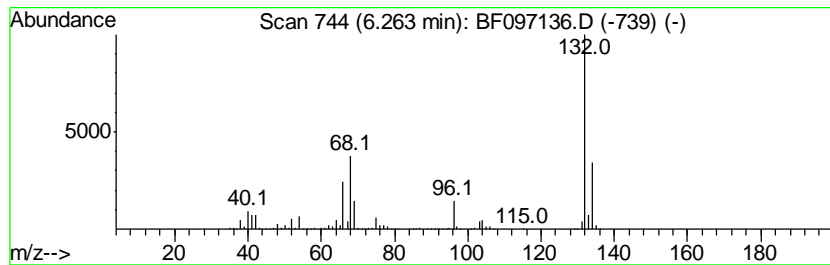
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF072517.M  
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TIC Library : C:\DATABASE\NIST11.L  
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 Peak Number 2 unknown6.26 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.26	70.75 ng	2375340	1,4-Dichlorobenzene-d4	6.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF072517.M  
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

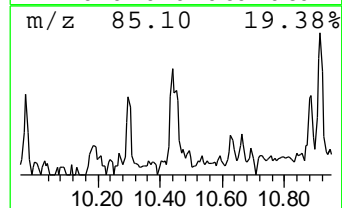
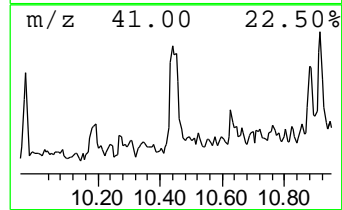
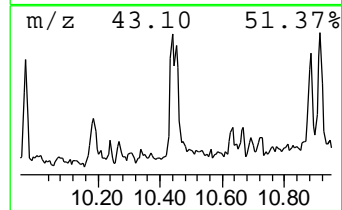
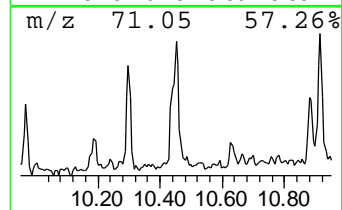
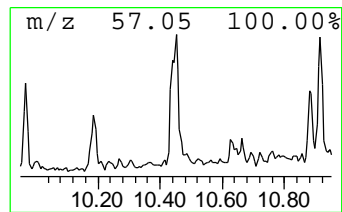
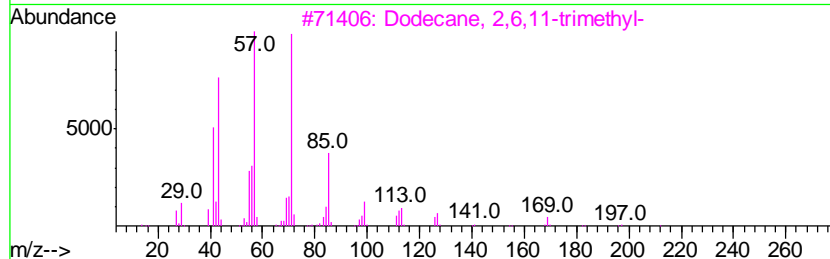
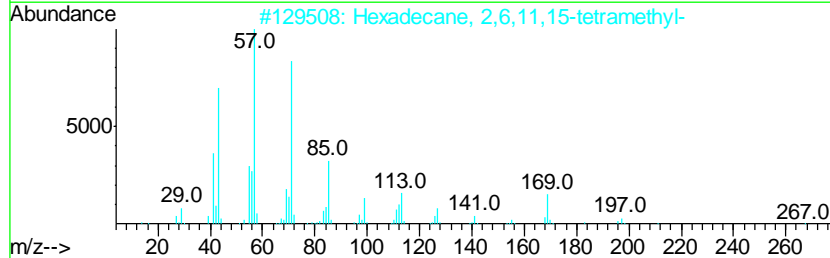
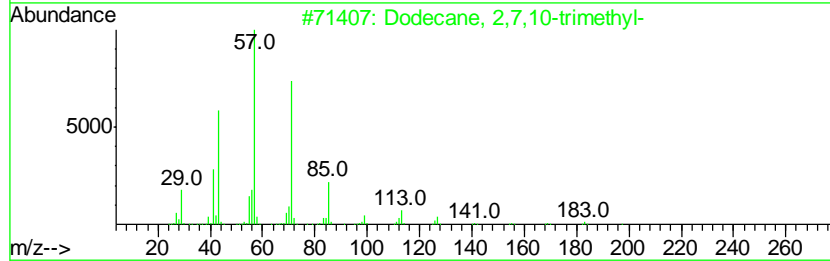
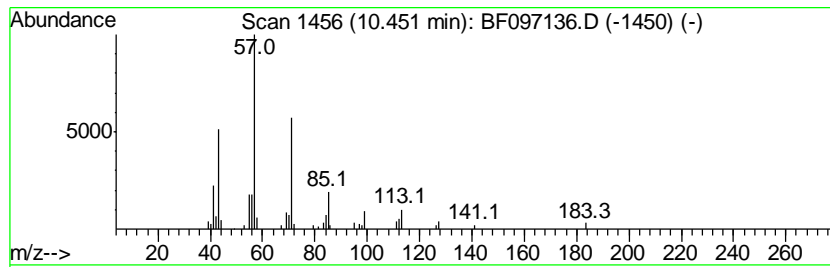
TIC Library : C:\DATABASE\NIST11.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 4 Dodecane, 2,7,10-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.45	2.71 ng	106430	Phenanthrene-d10	10.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	86
2		Hexadecane, 2,6,11,15-tetramethyl-	282	C20H42	000504-44-9	86
3		Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	80
4		Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	72
5		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	64



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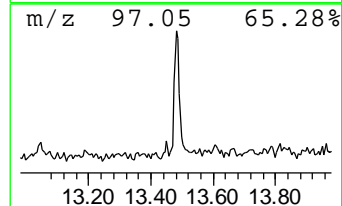
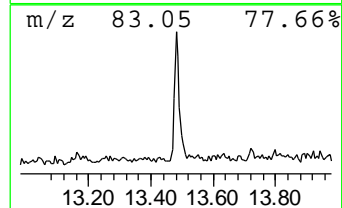
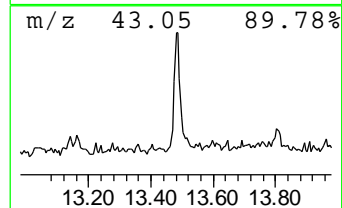
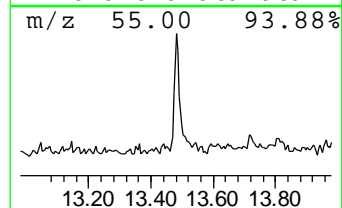
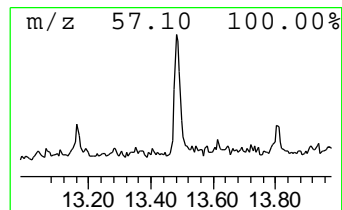
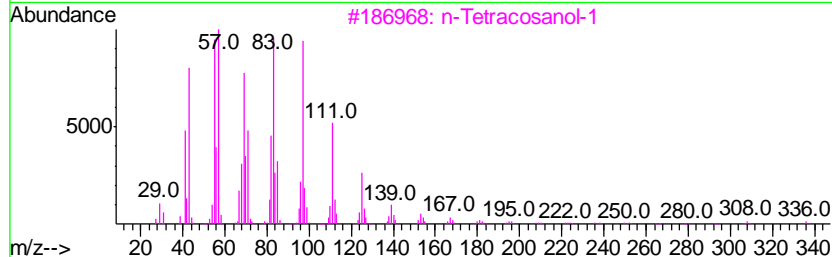
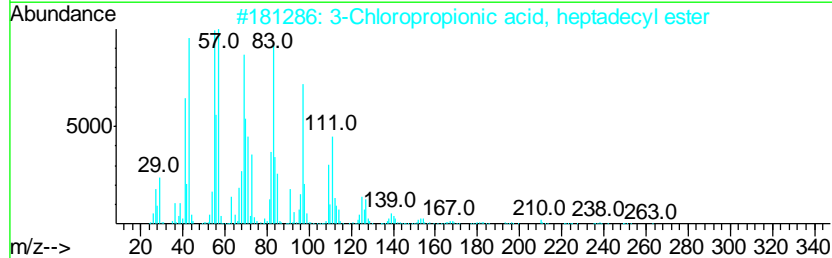
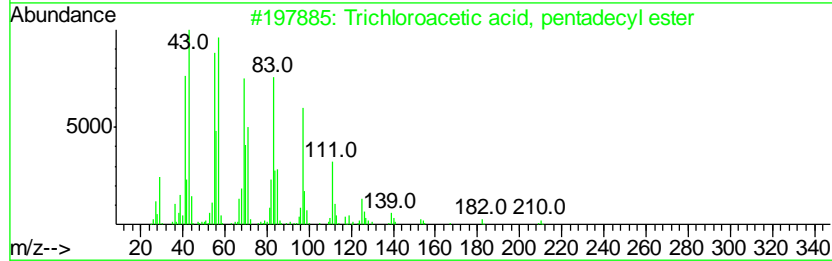
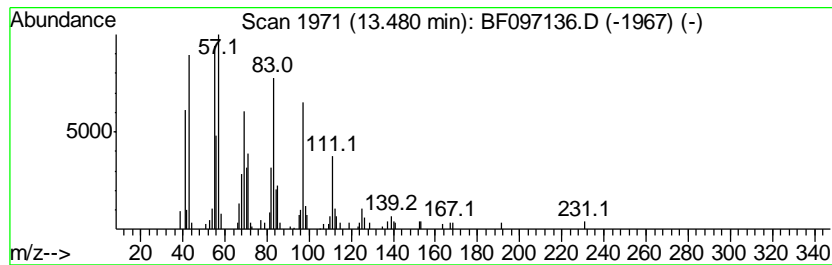
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 Peak Number 5 Trichloroacetic acid, penta... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.48	4.54 ng	143110	Chrysene-d12	13.61

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
2		3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4		5-Eicosene, (E)-	280	C20H40	074685-30-6	91
5		11-Tricosene	322	C23H46	052078-56-5	91



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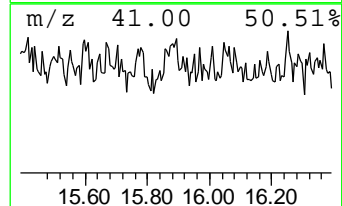
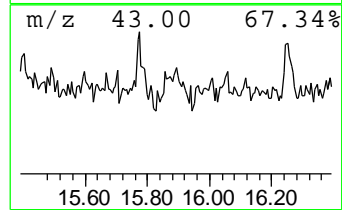
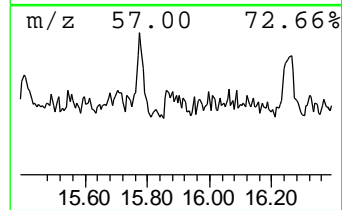
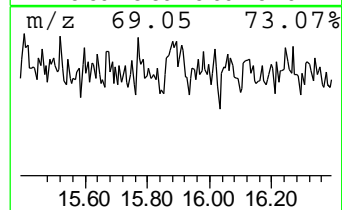
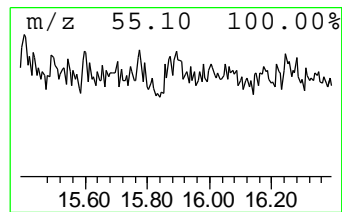
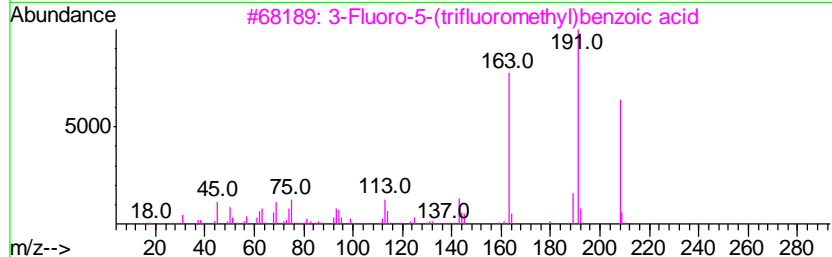
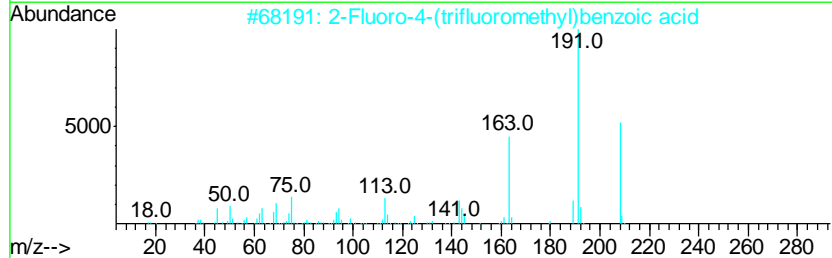
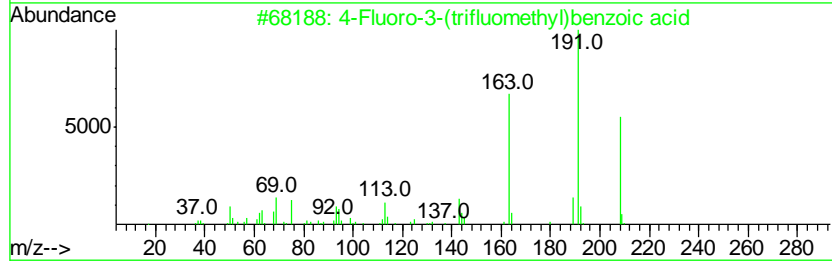
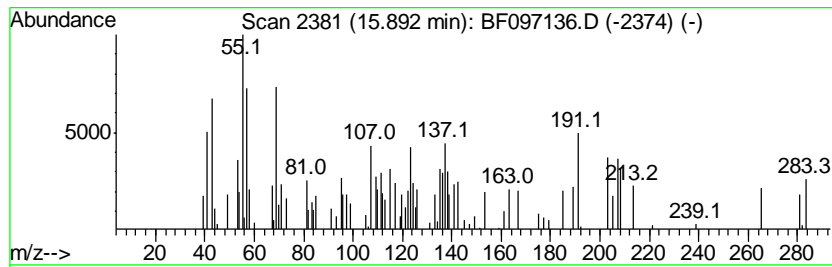
TIC Library : C:\DATABASE\NIST11.L  
 TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
 Peak Number 6 unknown15.89 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.89	3.60 ng	95714	Perylene-d12	14.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Fluoro-3-(trifluoromethyl)benzoi...	208	C8H4F4O2	067515-55-3	30
2		2-Fluoro-4-(trifluoromethyl)benz...	208	C8H4F4O2	115029-24-8	27
3		3-Fluoro-5-(trifluoromethyl)benz...	208	C8H4F4O2	161622-05-5	27
4		4-Fluoro-2-(trifluoromethyl)benz...	208	C8H4F4O2	1000342-47-8	27
5		3-Fluoro-5-trifluoromethylbenzam...	277	C13H15F4NO	1000358-14-1	25





Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF072717\  
Data File : BF097136.D  
Acq On : 27 Jul 2017 21:37  
Operator : SJ/JU  
Sample : I4422-13  
Misc :  
ALS Vial : 43 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
72-11940-COMP

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF072517.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.63	7.2	ng	241204	1	6.49	671482	20.0
unknown6.26	6.26	70.8	ng	2375340	1	6.49	671482	20.0
Dodecane, 2,7,10-...	10.45	2.7	ng	106430	4	10.99	784645	20.0
Trichloroacetic a...	13.48	4.5	ng	143110	5	13.61	631043	20.0
unknown15.89	15.89	3.6	ng	95714	6	14.96	532272	20.0