

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
 Data File : BF085523.D
 Acq On : 18 Mar 2016 7:08
 Operator : UM/SJ
 Sample : H1776-06
 Misc :
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 W170TH-SB-11(0.5-1.0)

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-BF031516.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	4.470	189	191	196	rBV	122054	186751	1.59%	0.319%
2	5.476	277	279	282	rBV	2489487	2522020	21.53%	4.311%
3	6.059	328	330	333	rVB	253064	279740	2.39%	0.478%
4	6.504	366	369	372	rVB	2277272	2521368	21.52%	4.310%
5	6.642	379	381	383	rBV	2919456	2683721	22.91%	4.587%
6	6.802	393	395	399	rBV	133230	146819	1.25%	0.251%
7	6.870	399	401	404	rVV	767136	765930	6.54%	1.309%
8	6.950	406	408	410	rBV	474682	472945	4.04%	0.808%
9	6.996	410	412	413	rVV	162346	164145	1.40%	0.281%
10	7.030	413	415	418	rVB	2529595	2285180	19.51%	3.906%
11	7.442	448	451	453	rBV	1921122	2005120	17.12%	3.427%
12	8.162	512	514	515	rVV	1193888	1051537	8.98%	1.797%
13	9.236	606	608	611	rBV	2716075	2469923	21.08%	4.222%
14	9.362	616	619	623	rVB	226462	243121	2.08%	0.416%
15	9.636	640	643	645	rVV	523293	635417	5.42%	1.086%
16	9.911	665	667	669	rBV	739880	1001824	8.55%	1.712%
17	10.345	704	705	709	rVB	122572	117953	1.01%	0.202%
18	10.699	734	736	739	rBV2	1321208	1680958	14.35%	2.873%
19	10.825	745	747	751	rBV	108376	173381	1.48%	0.296%
20	11.099	767	771	773	rVB	183115	231945	1.98%	0.396%
21	11.271	782	786	790	rBV3	90757	220714	1.88%	0.377%
22	11.374	793	795	801	rVV2	2738801	5094322	43.48%	8.708%
23	11.454	801	802	803	rVV	130012	154845	1.32%	0.265%
24	11.499	805	806	808	rVV	164099	164249	1.40%	0.281%
25	11.545	808	810	811	rVV	876862	845535	7.22%	1.445%
26	11.934	839	844	846	rBV2	1288500	1835179	15.66%	3.137%
27	11.968	846	847	850	rVB	169496	175299	1.50%	0.300%
28	12.608	901	903	904	rBV	391514	430180	3.67%	0.735%
29	12.642	904	906	909	rVV	807634	971702	8.29%	1.661%
30	12.711	911	912	916	rVB2	270888	309093	2.64%	0.528%
31	12.836	918	923	924	rBV	317107	341172	2.91%	0.583%
32	12.985	933	936	938	rVB	1962944	1830055	15.62%	3.128%
33	13.214	954	956	959	rVB2	151262	152831	1.30%	0.261%
34	13.557	984	986	988	rBV	382568	340975	2.91%	0.583%

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W170TH-SB-11(0.5-1.0)

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

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35	13.888	1012	1015	1017	rVB	808727	865740	7.39%	1.480%
36	14.037	1024	1028	1029	rBV2	761259	1041038	8.89%	1.779%
37	14.197	1040	1042	1045	rVB	681591	759552	6.48%	1.298%
38	14.380	1055	1058	1060	rBV2	63253	133549	1.14%	0.228%
39	14.505	1067	1069	1071	rVV	1014047	917691	7.83%	1.569%
40	14.802	1091	1095	1098	rBV	743094	847011	7.23%	1.448%
41	15.054	1115	1117	1121	rBV	159865	314560	2.69%	0.538%
42	15.134	1121	1124	1128	rVB	716211	860308	7.34%	1.471%
43	15.351	1140	1143	1146	rVB	106709	160916	1.37%	0.275%
44	15.408	1146	1148	1151	rBV	133232	161923	1.38%	0.277%
45	15.465	1151	1153	1155	rBV	471671	833006	7.11%	1.424%
46	15.500	1155	1156	1161	rVB	469222	454129	3.88%	0.776%
47	15.923	1190	1193	1195	rBV	350717	553735	4.73%	0.947%
48	16.174	1211	1215	1221	rVB6	59272	204600	1.75%	0.350%
49	16.403	1232	1235	1239	rBV	157192	306355	2.62%	0.524%
50	16.974	1282	1285	1289	rBV	121694	259974	2.22%	0.444%
51	17.454	1323	1327	1331	rBV4	56353	195151	1.67%	0.334%
52	17.534	1331	1334	1339	rVB4	93658	236015	2.01%	0.403%
53	17.648	1340	1344	1348	rBV2	88012	221200	1.89%	0.378%
54	17.740	1348	1352	1357	rBV	325719	909402	7.76%	1.554%
55	18.003	1370	1375	1376	rBV	139199	329781	2.81%	0.564%
56	18.106	1376	1384	1392	rVV3	2690176	11715160	100.00%	20.025%
57	18.231	1392	1395	1405	rVB2	170484	668091	5.70%	1.142%
58	18.437	1410	1413	1421	rVB2	71207	249231	2.13%	0.426%
59	18.871	1446	1451	1458	rVB3	75806	246393	2.10%	0.421%
60	19.454	1497	1502	1509	rVB3	163346	552568	4.72%	0.945%

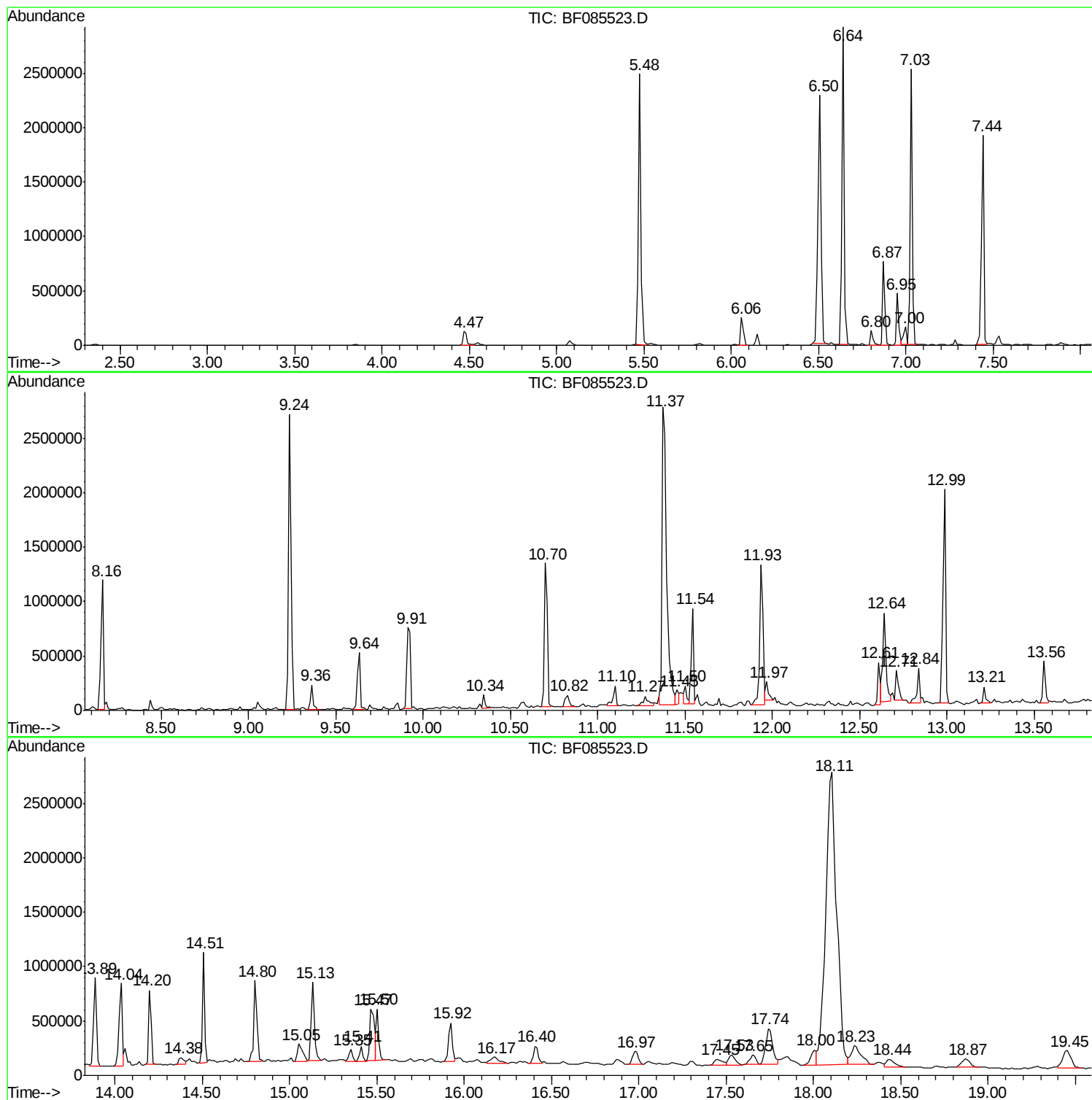
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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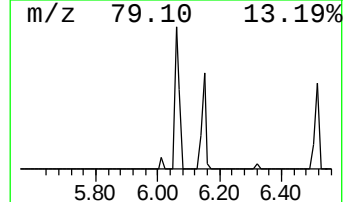
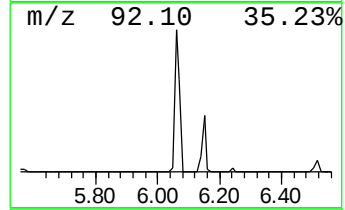
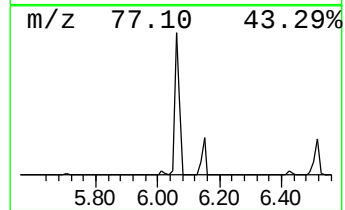
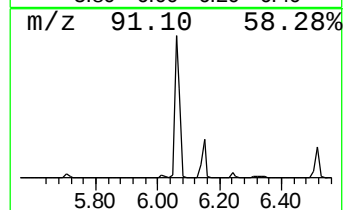
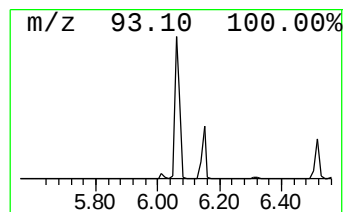
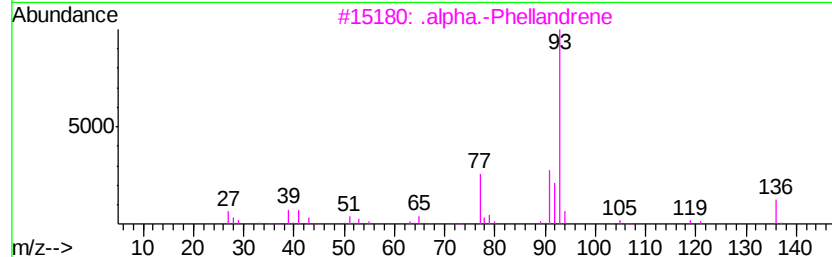
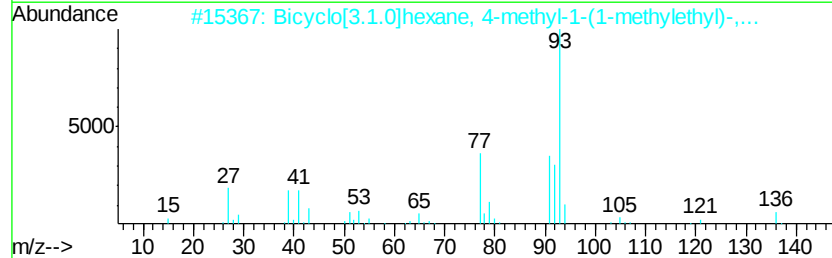
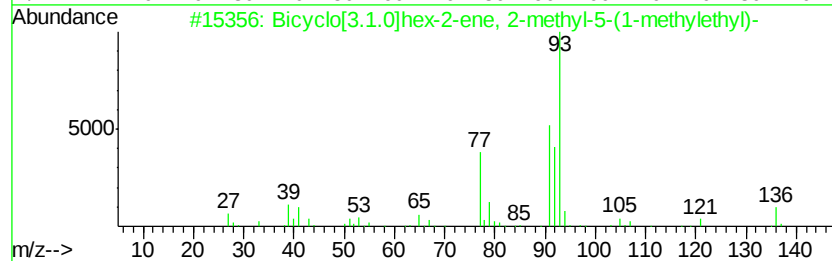
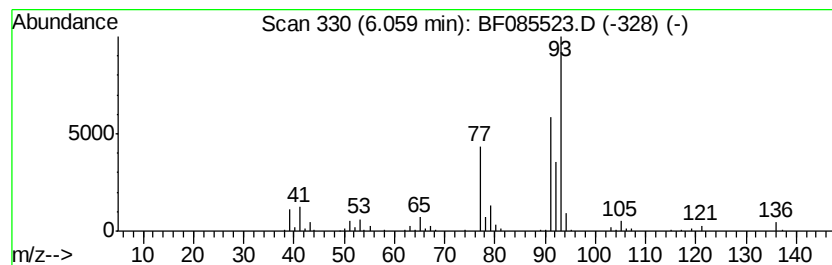
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Bicyclo[3.1.0]hex-2-ene, 2-... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.06	7.30 ng	279740	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bicyclo[3.1.0]hex-2-ene, 2-methy...	136	C10H16	002867-05-2	91
2		Bicyclo[3.1.0]hexane, 4-methyl-1...	136	C10H16	058037-87-9	83
3		.alpha.-Phellandrene	136	C10H16	000099-83-2	83
4		1,4-Methano-1H-Cyclopropa[d]pyri...	136	C8H12N2	109746-10-3	72
5		Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	72



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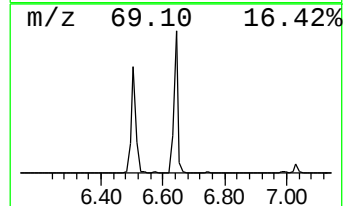
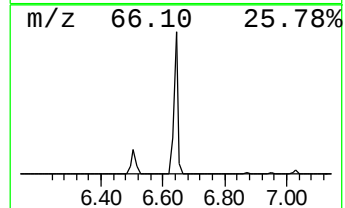
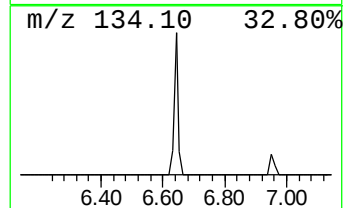
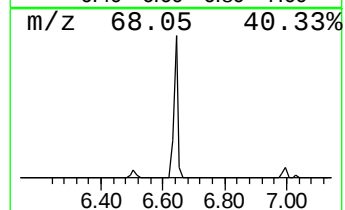
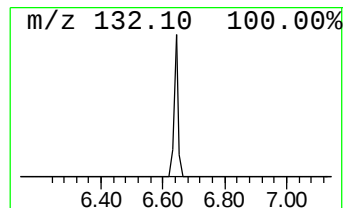
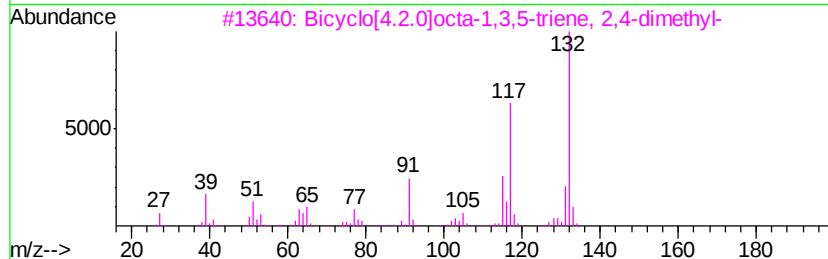
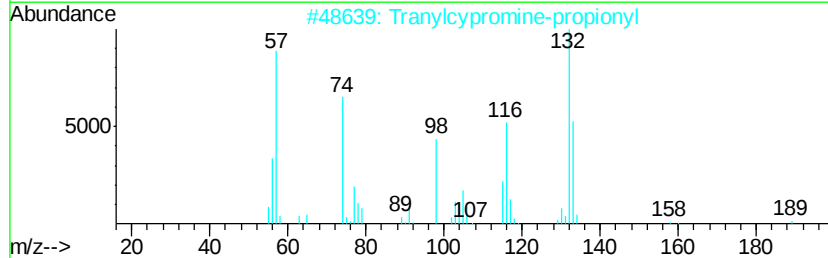
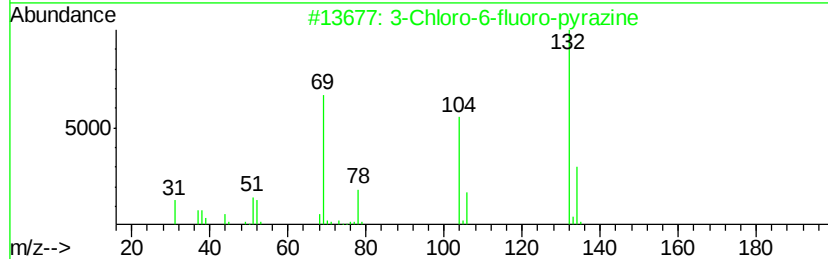
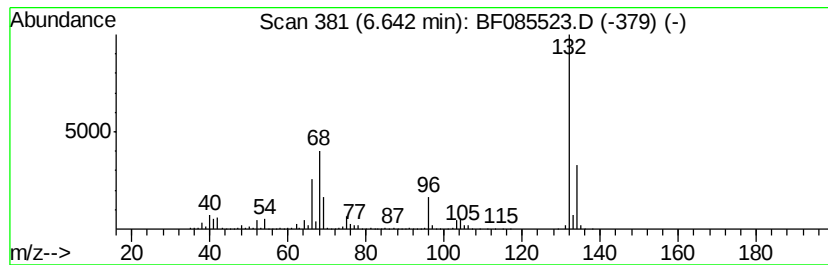
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.64 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	70.08 ng	2683720	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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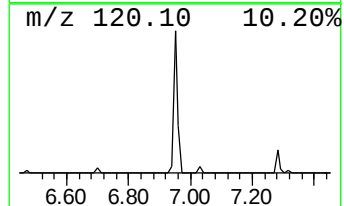
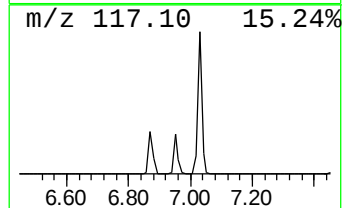
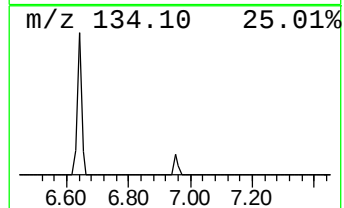
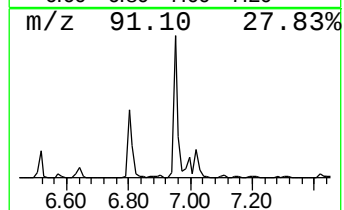
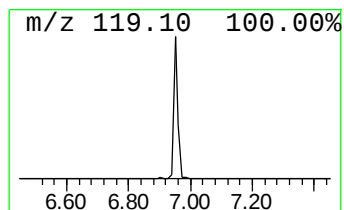
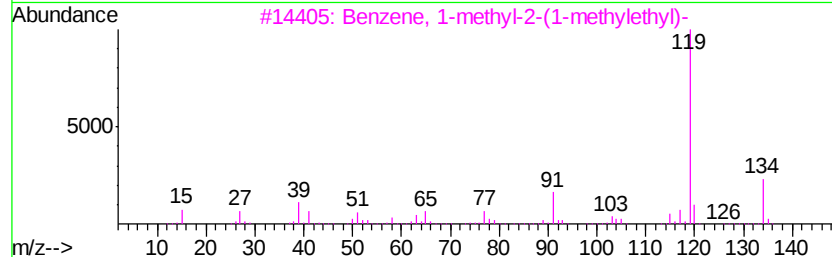
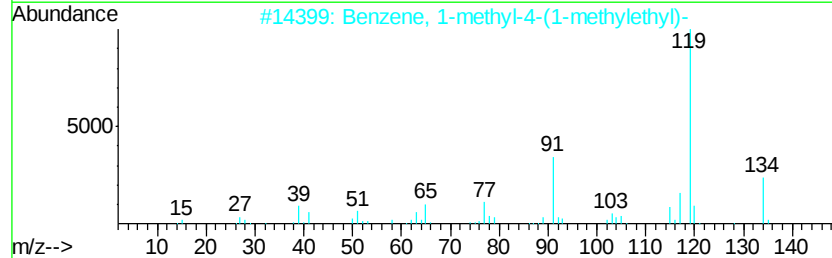
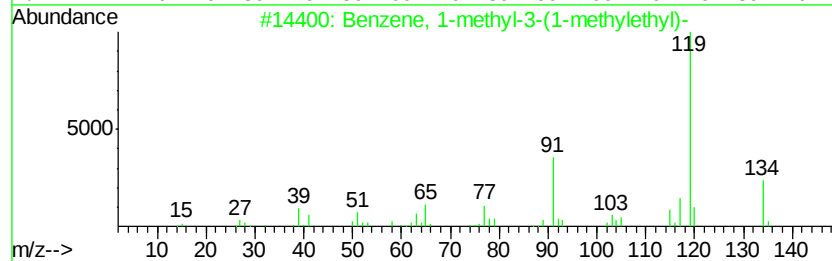
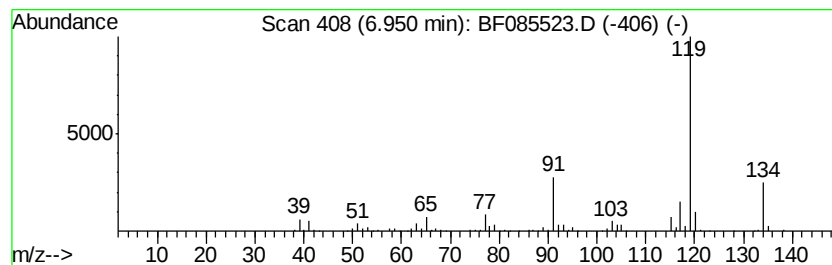
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzene, 1-methyl-3-(1-meth... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.95	12.35 ng	472945	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
2		Benzene, 1-methyl-4-(1-methyleth...	134	C10H14	000099-87-6	95
3		Benzene, 1-methyl-2-(1-methyleth...	134	C10H14	000527-84-4	94
4		Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	91
5		Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	91



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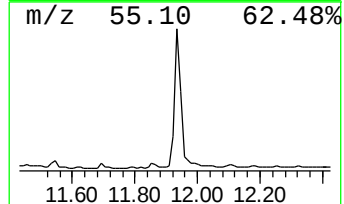
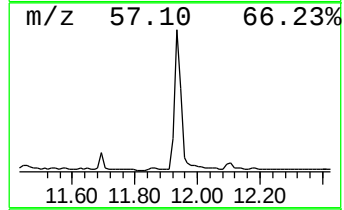
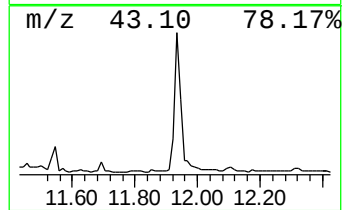
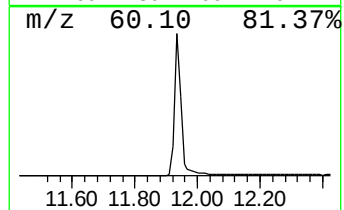
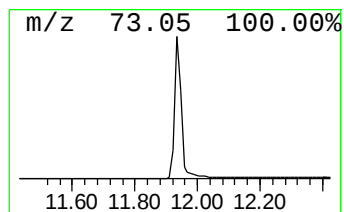
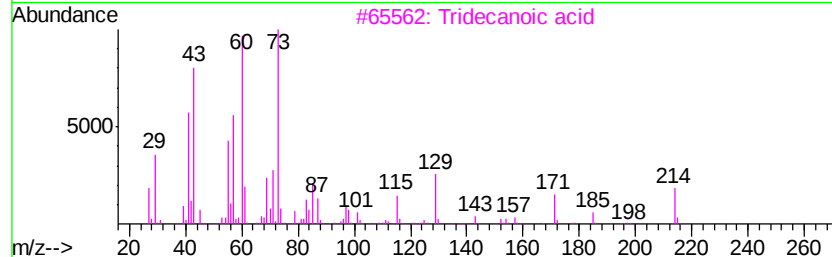
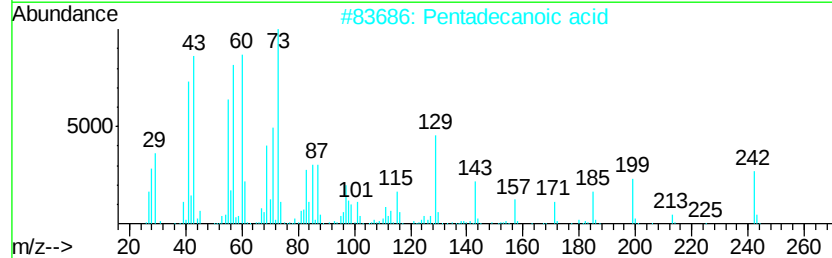
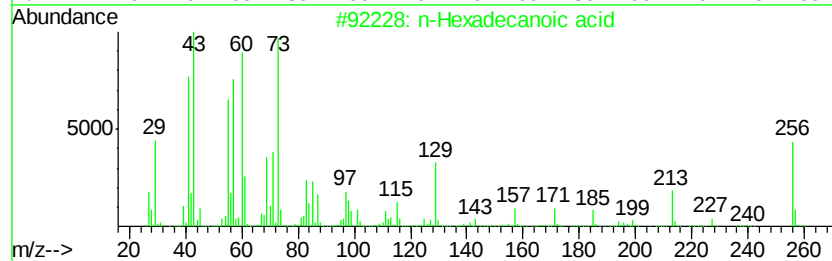
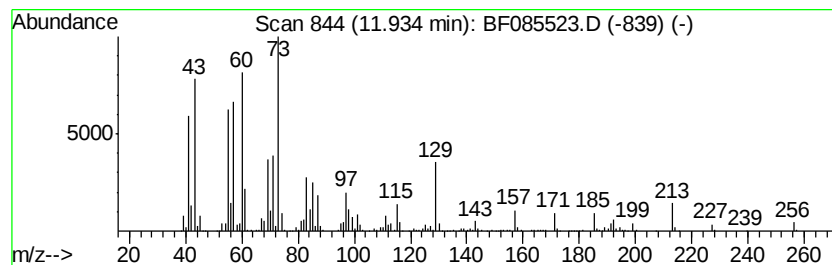
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	7.20 ng	1835180	Phenanthrene-d10	11.40

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3		Tridecanoic acid	214	C13H26O2	000638-53-9	81
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5		Estra-1,3,5(10)-trien-17.beta.-ol	256	C18H24O	002529-64-8	30



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W170TH-SB-11(0.5-1.0)

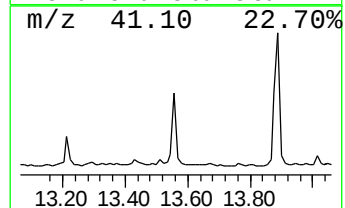
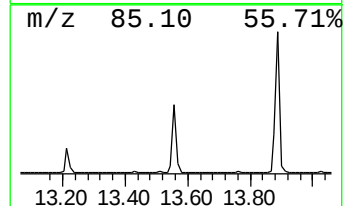
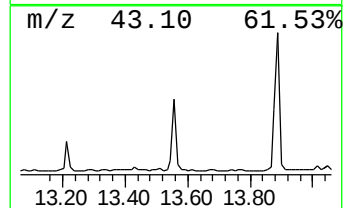
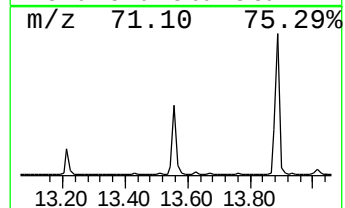
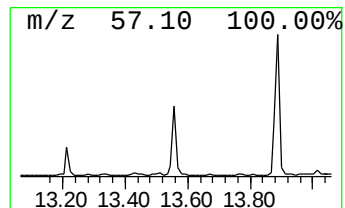
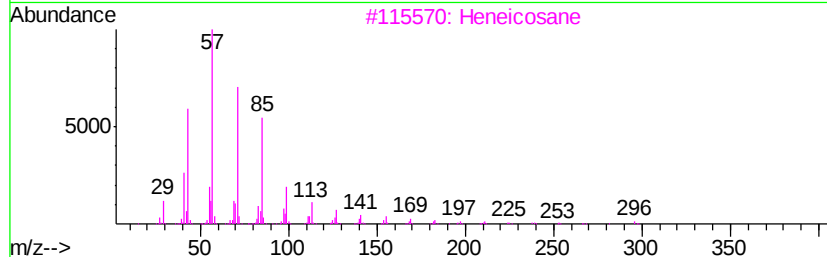
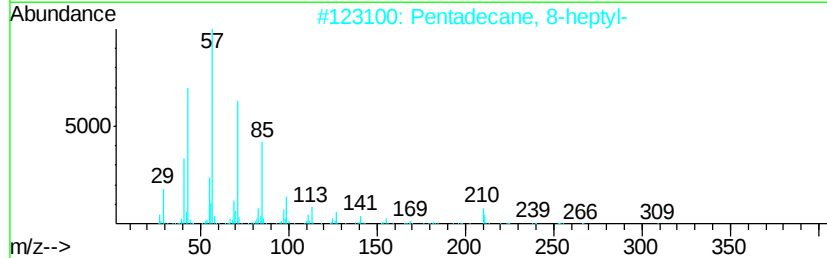
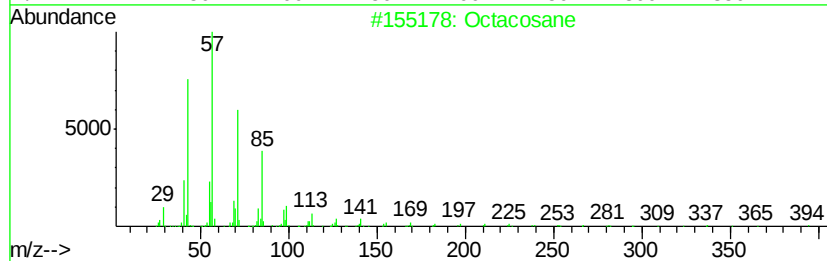
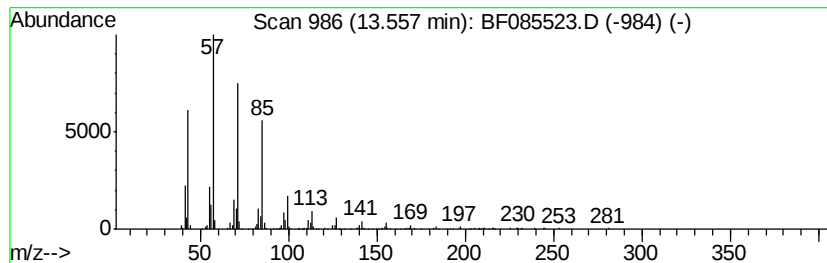
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octacosane Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.56	6.55 ng	340975	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Hexadecane	226	C16H34	000544-76-3	90
5		Pentacosane	352	C25H52	000629-99-2	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
Data File : BF085523.D
Acq On : 18 Mar 2016 7:08
Operator : UM/SJ
Sample : H1776-06
Misc :
ALS Vial : 43 Sample Multiplier: 1

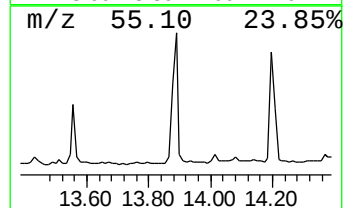
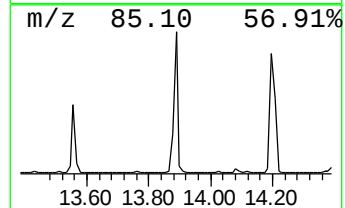
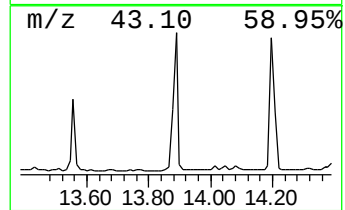
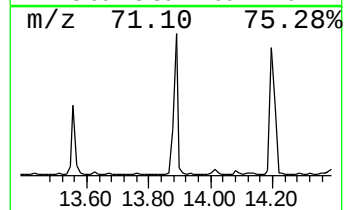
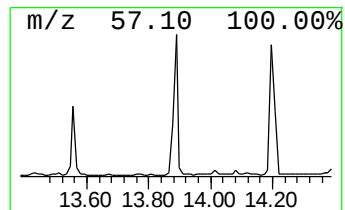
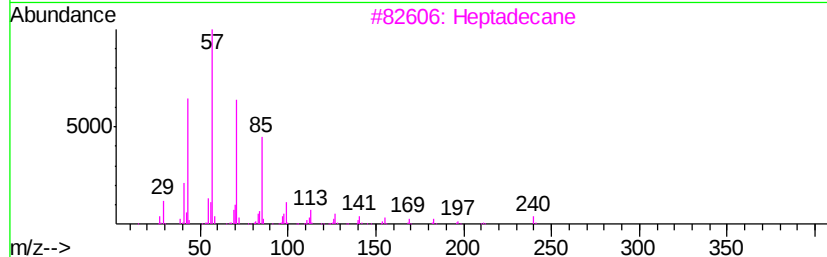
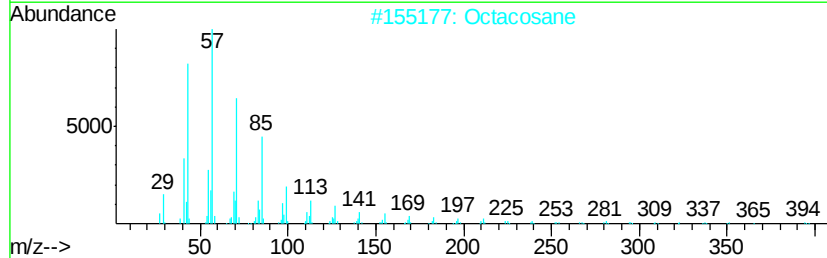
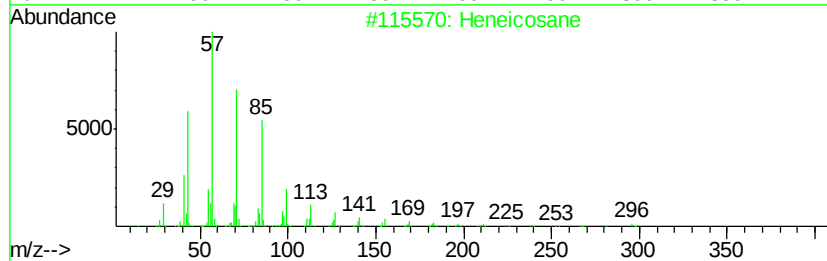
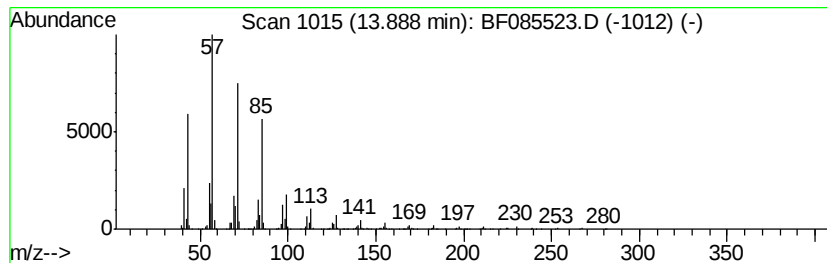
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.89	16.63 ng	865740	Chrysene-d12	14.04	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Heptadecane	240	C17H36	000629-78-7	90
4	Hexadecane	226	C16H34	000544-76-3	87
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
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Operator : UM/SJ
Sample : H1776-06
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Instrument :
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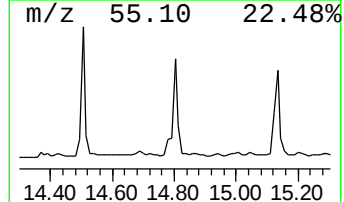
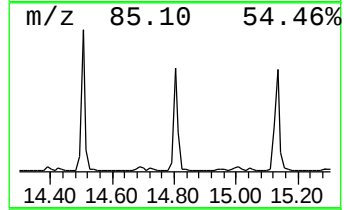
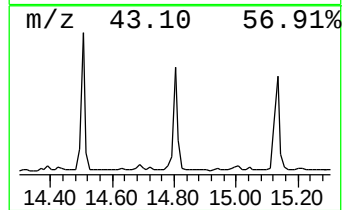
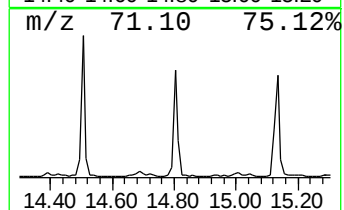
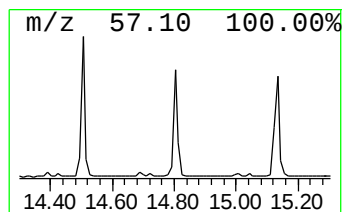
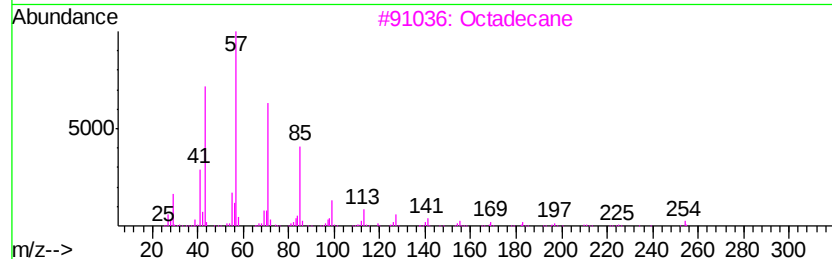
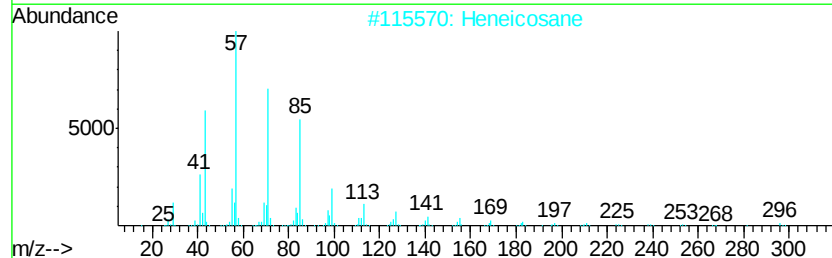
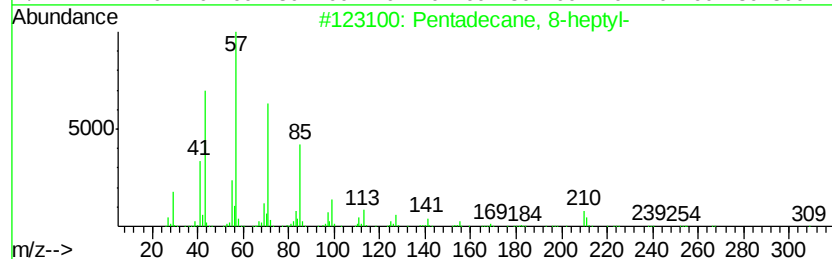
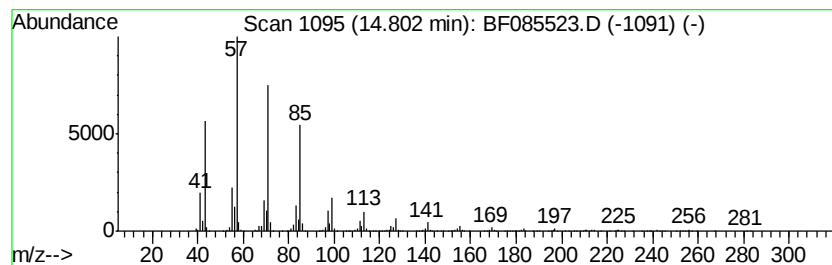
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Pentadecane, 8-heptyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	20.34 ng	847011	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Octadecane	254	C18H38	000593-45-3	86
4		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
5		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
Data File : BF085523.D
Acq On : 18 Mar 2016 7:08
Operator : UM/SJ
Sample : H1776-06
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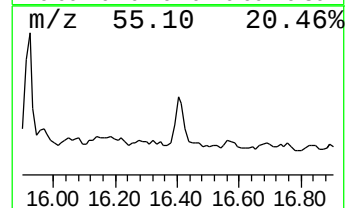
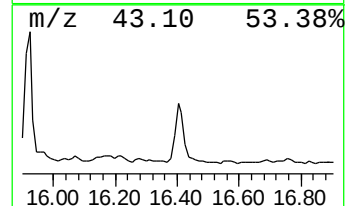
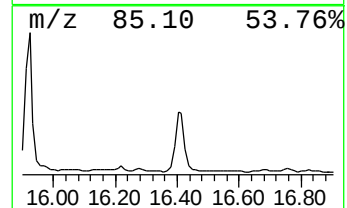
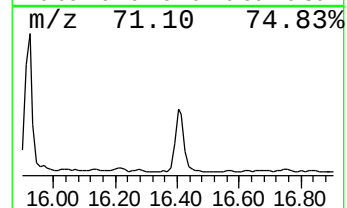
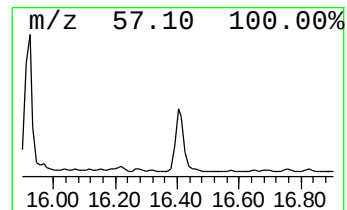
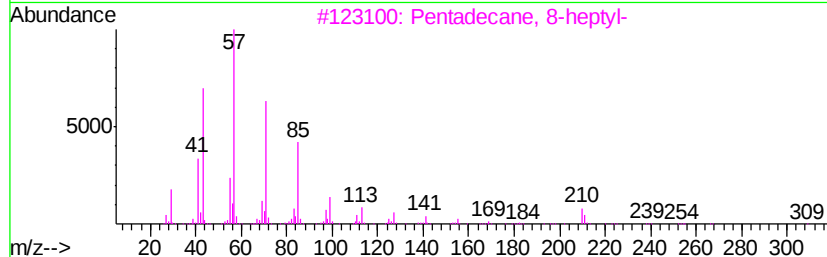
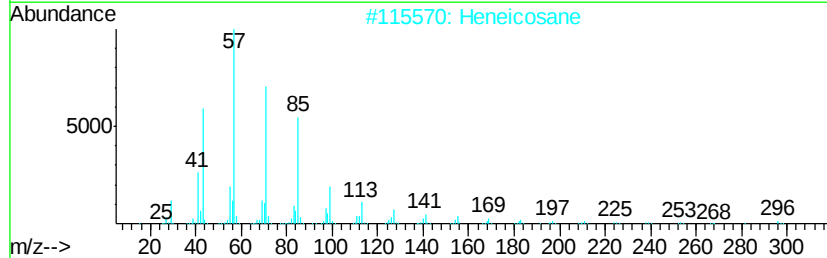
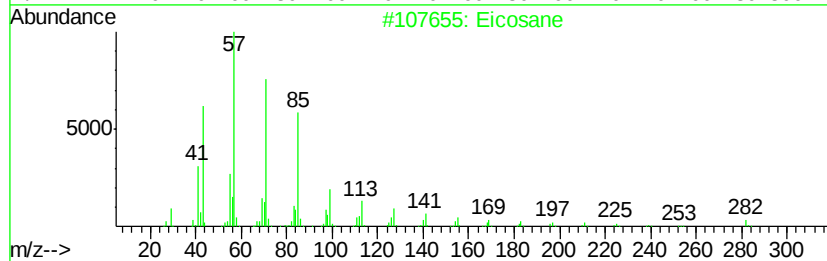
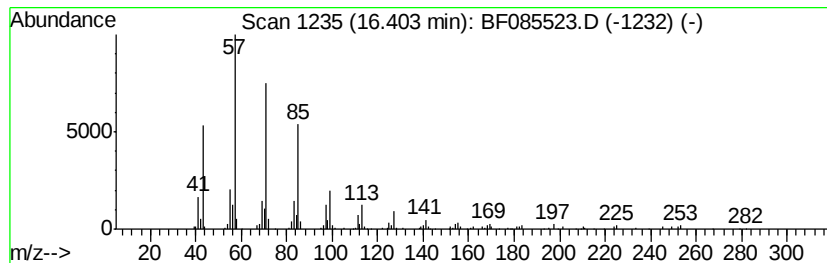
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Eicosane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.40	7.36 ng	306355	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	94
2		Heneicosane	296	C21H44	000629-94-7	91
3		Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91
4		Tetratriacontane	479	C34H70	014167-59-0	91
5		Octacosane	394	C28H58	000630-02-4	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
Data File : BF085523.D
Acq On : 18 Mar 2016 7:08
Operator : UM/SJ
Sample : H1776-06
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Instrument :
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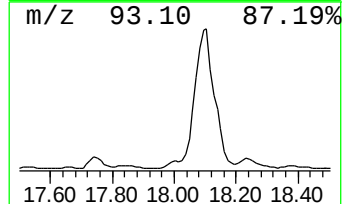
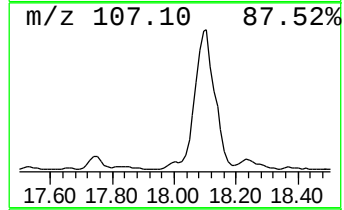
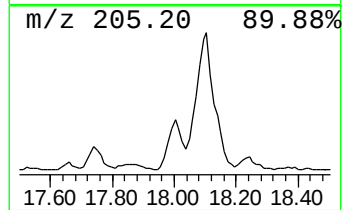
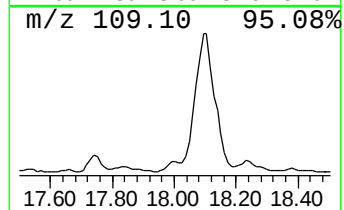
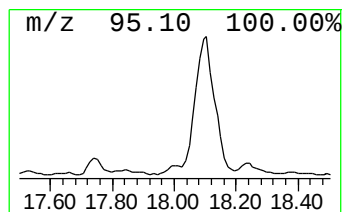
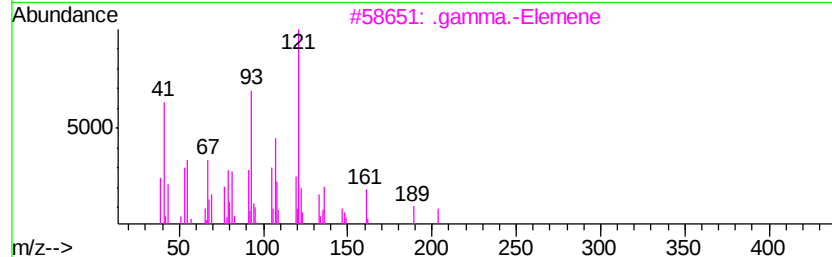
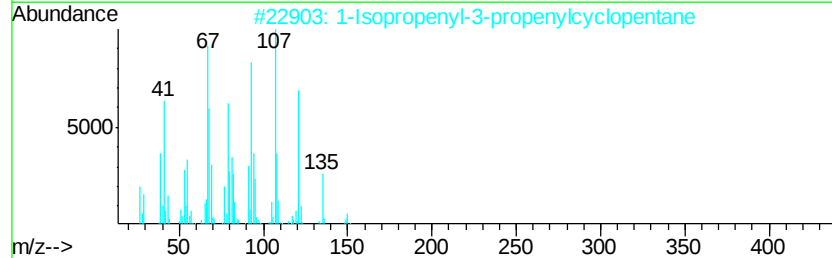
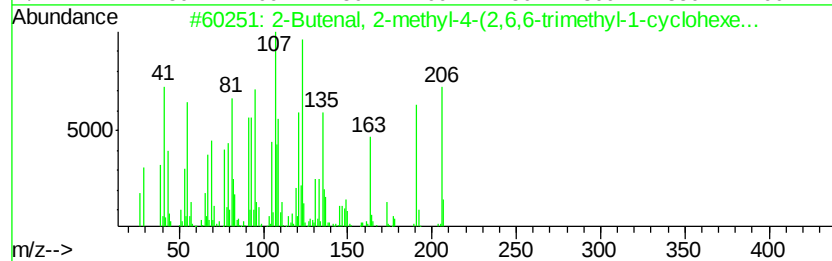
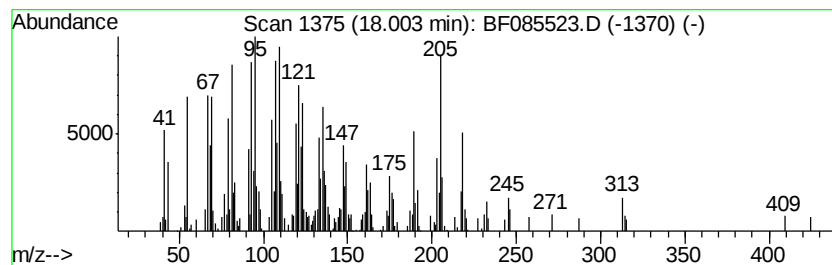
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown18.00 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.00	7.92 ng	329781	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Butenal, 2-methyl-4-(2,6,6-tri...	206	C14H22O	003155-71-3	49
2		1-Isopropenyl-3-propenylcyclopent...	150	C11H18	1000192-81-2	47
3		.gamma.-Elemene	204	C15H24	030824-67-0	44
4		Azulene, 1,2,3,5,6,7,8,8a-octahy...	204	C15H24	003691-11-0	42
5		Eudesma-4(14),11-diene	204	C15H24	1000152-04-3	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
Data File : BF085523.D
Acq On : 18 Mar 2016 7:08
Operator : UM/SJ
Sample : H1776-06
Misc :
ALS Vial : 43 Sample Multiplier: 1

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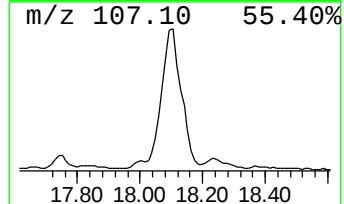
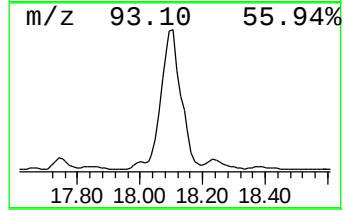
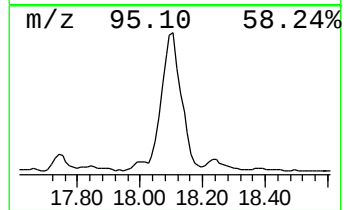
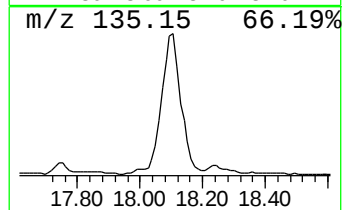
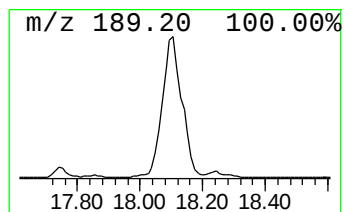
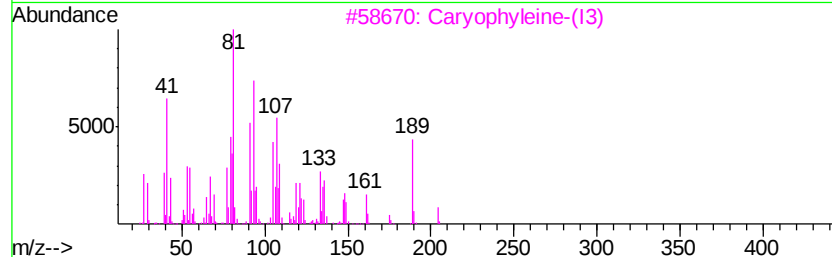
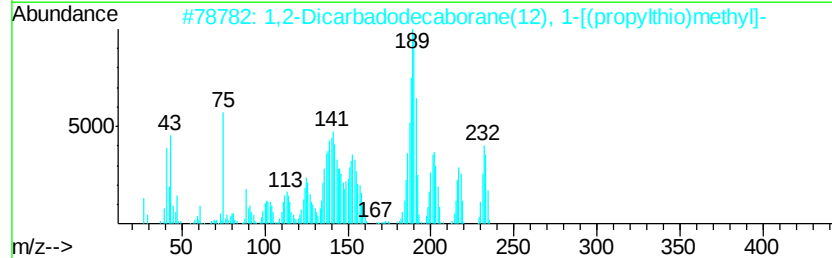
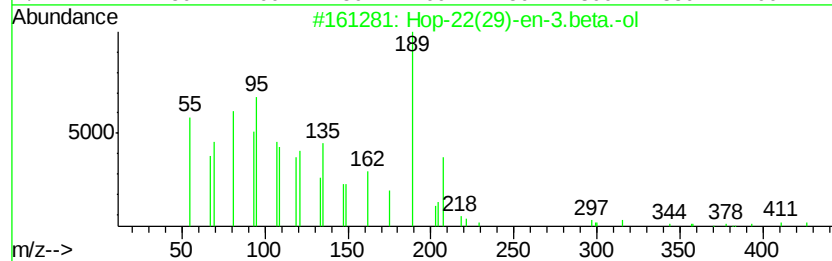
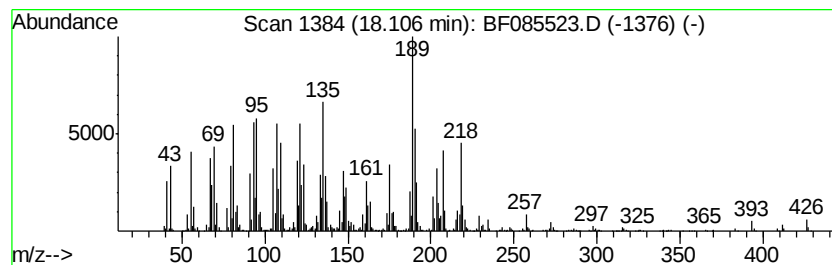
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Hop-22(29)-en-3.beta.-ol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.11	281.27 ng	11715200	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hop-22(29)-en-3.beta.-ol	426	C30H50O	058801-23-3	94
2		1,2-Dicarbododecaborane(12), 1-[...]	234	C6H20B10S	062906-36-9	94
3		Caryophyllene-(I3)	204	C15H24	136296-37-2	27
4		2,6,10-Cycloundecatrien-1-one, 2...	218	C15H22O	000471-05-6	22
5		Cycloheptane, 4-methylene-1-meth...	204	C15H24	1000159-38-5	20



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
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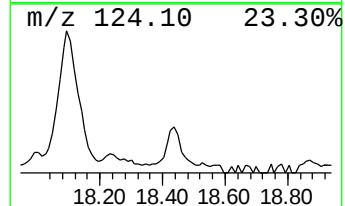
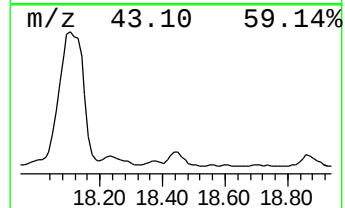
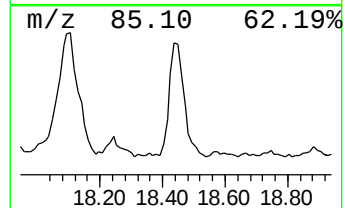
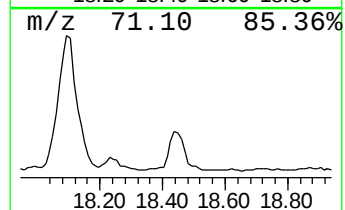
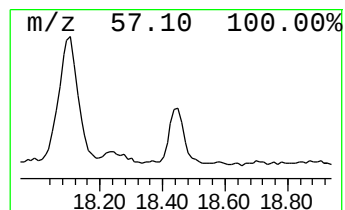
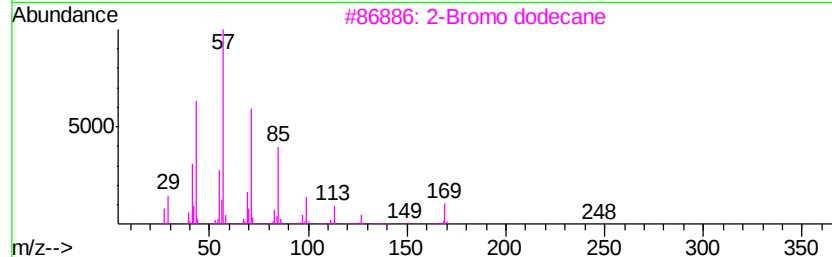
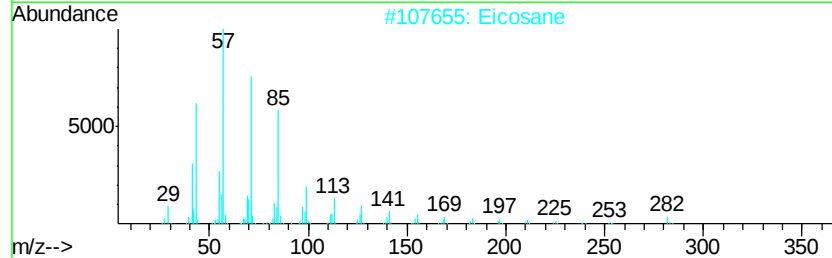
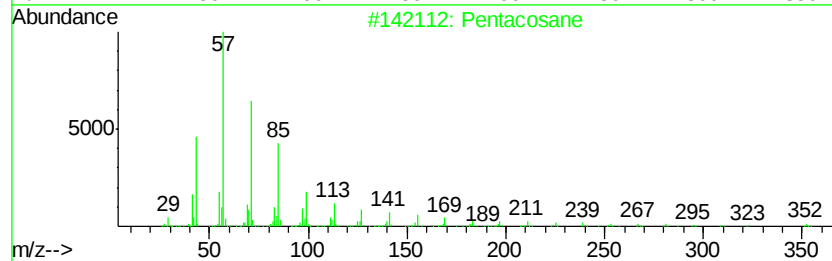
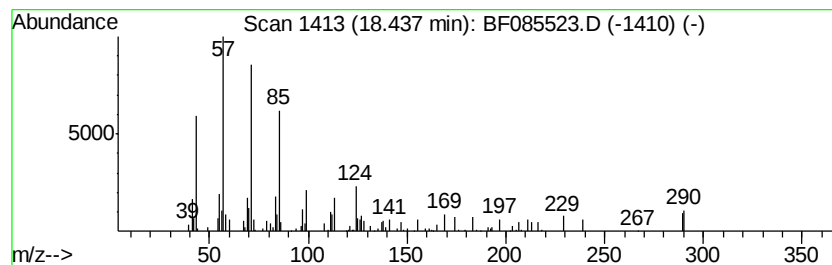
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Pentacosane Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.44	5.98 ng	249231	Perylene-d12	15.47
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Pentacosane	352 C25H52	000629-99-2	64
2	Eicosane	282 C20H42	000112-95-8	58
3	2-Bromo dodecane	248 C12H25Br	013187-99-0	58
4	Heptadecane	240 C17H36	000629-78-7	58
5	Hexacosane	366 C26H54	000630-01-3	58



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
Data File : BF085523.D
Acq On : 18 Mar 2016 7:08
Operator : UM/SJ
Sample : H1776-06
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W170TH-SB-11(0.5-1.0)

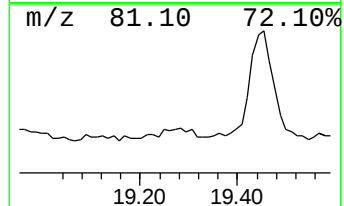
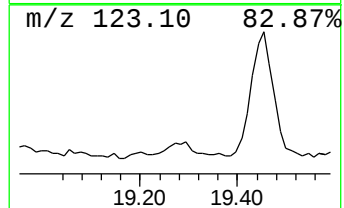
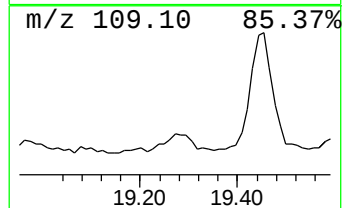
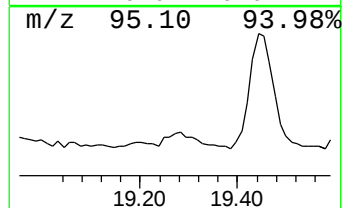
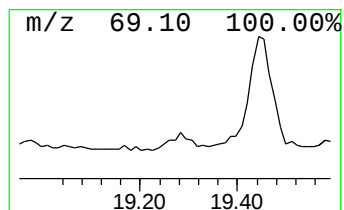
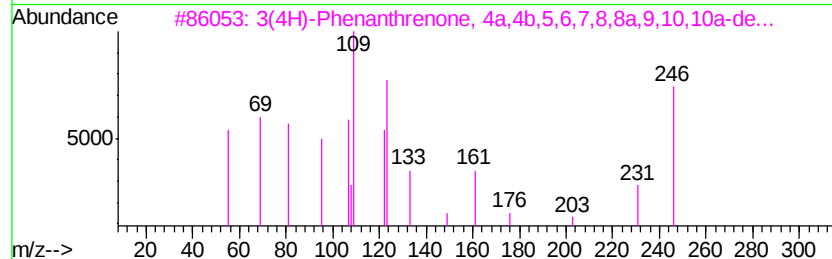
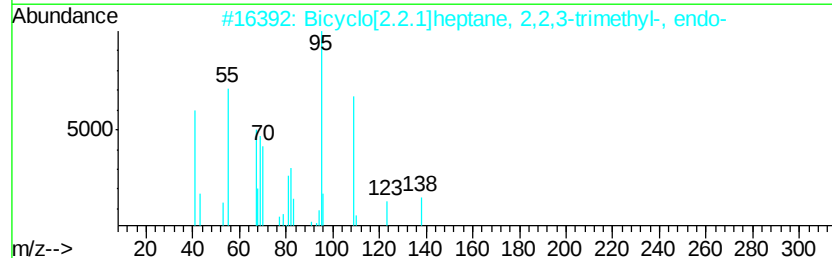
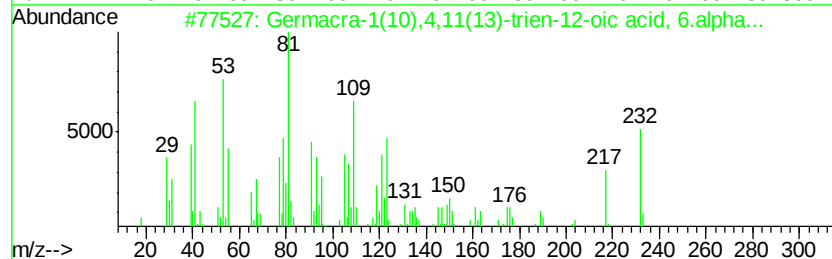
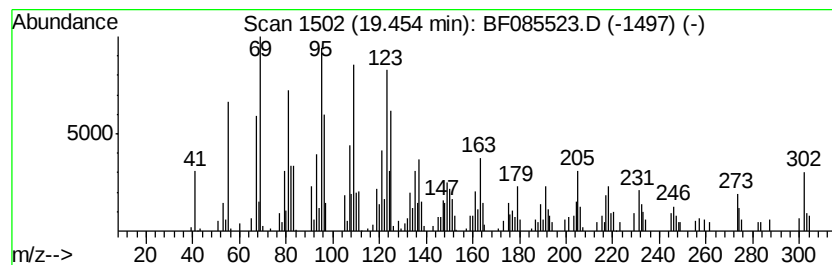
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 unknown19.45 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.45	13.27 ng	552568	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Germacra-1(10),4,11(13)-trien-12...	232	C15H20O2	000553-21-9	46
2		Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-40-7	38
3		3(4H)-Phenanthrenone, 4a,4b,5,6,...	246	C17H26O	057684-12-5	30
4		2-Cyclohexene-1-carboxaldehyde, ...	220	C15H24O	056772-07-7	25
5		13,17-Seco-5.alpha.-pregn-13(18)...	302	C21H34O	031239-27-7	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
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 Misc :
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 W170TH-SB-11(0.5-1.0)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.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
Bicyclo[3.1.0]hex...	6.06	7.3	ng	279740	1	6.87	765930	20.0
unknown6.64	6.64	70.1	ng	2683720	1	6.87	765930	20.0
Benzene, 1-methyl...	6.95	12.4	ng	472945	1	6.87	765930	20.0
n-Hexadecanoic acid	11.93	7.2	ng	1835180	4	11.40	5094320	20.0
Octacosane	13.56	6.5	ng	340975	5	14.04	1041040	20.0
Heneicosane	13.89	16.6	ng	865740	5	14.04	1041040	20.0
Pentadecane, 8-he...	14.80	20.3	ng	847011	6	15.47	833006	20.0
Eicosane	16.40	7.4	ng	306355	6	15.47	833006	20.0
2(1H)Naphthalenon...	17.74	21.8	ng	909402	6	15.47	833006	20.0
unknown18.00	18.00	7.9	ng	329781	6	15.47	833006	20.0
Hop-22(29)-en-3.b...	18.11	281.3	ng	11715200	6	15.47	833006	20.0
Pentacosane	18.44	6.0	ng	249231	6	15.47	833006	20.0
unknown19.45	19.45	13.3	ng	552568	6	15.47	833006	20.0