

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100317\
 Data File : BF099040.D
 Acq On : 3 Oct 2017 19:53
 Operator : SJ/JU
 Sample : I5496-04
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PAMT-COMP-E

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-BF092317.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	2.152	7	11	30	rVB	463085	673935	58.05%	5.124%
2	2.281	30	33	38	rVB2	21695	32723	2.82%	0.249%
3	5.081	506	509	519	rVB	364892	358891	30.91%	2.729%
4	5.351	552	555	559	rVB	33749	29305	2.52%	0.223%
5	5.481	574	577	581	rBV	350805	293008	25.24%	2.228%
6	5.822	632	635	641	rVB	21348	19261	1.66%	0.146%
7	6.175	691	695	697	rBV	14571	13790	1.19%	0.105%
8	6.487	745	748	754	rBV2	306633	367350	31.64%	2.793%
9	6.634	769	773	777	rBV	621362	512986	44.19%	3.900%
10	6.716	781	787	789	rBV	20506	20228	1.74%	0.154%
11	6.869	810	813	817	rBV	893484	779584	67.15%	5.927%
12	7.028	836	840	843	rVB	926284	793801	68.37%	6.035%
13	7.428	904	908	912	rVB	744945	630612	54.32%	4.795%
14	7.504	918	921	927	rBV3	15371	16753	1.44%	0.127%
15	7.610	937	939	942	rVB	15308	12772	1.10%	0.097%
16	8.151	1027	1031	1035	rBV	1243512	1058181	91.15%	8.045%
17	8.645	1111	1115	1119	rVB2	10748	14758	1.27%	0.112%
18	8.775	1134	1137	1140	rBV	16536	15459	1.33%	0.118%
19	9.228	1209	1214	1217	rBV	1271169	1160956	100.00%	8.827%
20	9.304	1223	1227	1230	rBV2	13971	16637	1.43%	0.126%
21	9.616	1276	1280	1283	rBV	425782	342972	29.54%	2.608%
22	9.716	1293	1297	1302	rVB3	21664	23959	2.06%	0.182%
23	9.780	1303	1308	1312	rBV2	18298	24811	2.14%	0.189%
24	9.828	1312	1316	1319	rVB	32496	37825	3.26%	0.288%
25	9.910	1325	1330	1333	rBV	1298582	1147161	98.81%	8.722%
26	9.992	1342	1344	1351	rVB3	23859	24022	2.07%	0.183%
27	10.069	1351	1357	1358	rBV2	11152	15655	1.35%	0.119%
28	10.151	1368	1371	1375	rBV2	19519	19972	1.72%	0.152%
29	10.316	1395	1399	1404	rBV2	282541	291225	25.08%	2.214%
30	10.551	1434	1439	1441	rBV	48711	55424	4.77%	0.421%
31	10.633	1451	1453	1457	rVB4	16641	14397	1.24%	0.109%
32	10.669	1457	1459	1460	rBV2	19477	13128	1.13%	0.100%
33	10.692	1460	1463	1466	rVV	232072	181827	15.66%	1.382%
34	10.804	1479	1482	1491	rBV	143769	184036	15.85%	1.399%

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100317\
 Data File : BF099040.D
 Acq On : 3 Oct 2017 19:53
 Operator : SJ/JU
 Sample : I5496-04
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PAMT-COMP-E

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-BF092317.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	10.904	1496	1499	1501	rVB	14883	12566	1.08%	0.096%
36	10.992	1511	1514	1516	rBV2	20687	21306	1.84%	0.162%
37	11.127	1533	1537	1539	rBV	14253	14444	1.24%	0.110%
38	11.251	1555	1558	1560	rBV	89236	69581	5.99%	0.529%
39	11.280	1560	1563	1569	rVB2	45405	51929	4.47%	0.395%
40	11.339	1569	1573	1577	rVB5	16579	22436	1.93%	0.171%
41	11.392	1578	1582	1586	rBV	1224592	1069528	92.12%	8.132%
42	11.598	1614	1617	1618	rBV2	12767	12601	1.09%	0.096%
43	11.674	1628	1630	1636	rVB	28678	27092	2.33%	0.206%
44	11.939	1668	1675	1680	rBV8	10246	22585	1.95%	0.172%
45	12.080	1697	1699	1705	rVB	24217	19629	1.69%	0.149%
46	12.239	1721	1726	1731	rBV7	8762	12656	1.09%	0.096%
47	12.863	1829	1832	1835	rVB	36115	32406	2.79%	0.246%
48	12.974	1847	1851	1854	rVB	914351	754060	64.95%	5.733%
49	13.433	1927	1929	1935	rVB6	14851	21072	1.82%	0.160%
50	13.521	1942	1944	1949	rBV4	16101	17998	1.55%	0.137%
51	13.863	1998	2002	2009	rBV2	84895	107664	9.27%	0.819%
52	14.004	2023	2026	2027	rBV	61164	55811	4.81%	0.424%
53	14.027	2027	2030	2034	rVB	670007	634248	54.63%	4.822%
54	14.645	2133	2135	2139	rVB2	17868	17618	1.52%	0.134%
55	14.868	2169	2173	2189	rVB	87184	167121	14.40%	1.271%
56	15.133	2215	2218	2222	rVB2	14074	14866	1.28%	0.113%
57	15.504	2276	2281	2288	rBV	494330	579386	49.91%	4.405%
58	15.951	2354	2357	2363	rVB2	16926	21425	1.85%	0.163%
59	16.215	2397	2402	2412	rVB2	7980	24014	2.07%	0.183%
60	16.456	2437	2443	2455	rBV9	28286	65957	5.68%	0.501%
61	17.056	2540	2545	2552	rVB8	12533	27315	2.35%	0.208%
62	17.568	2627	2632	2636	rBV4	21822	44622	3.84%	0.339%
63	18.603	2805	2808	2814	rVB6	8631	13123	1.13%	0.100%

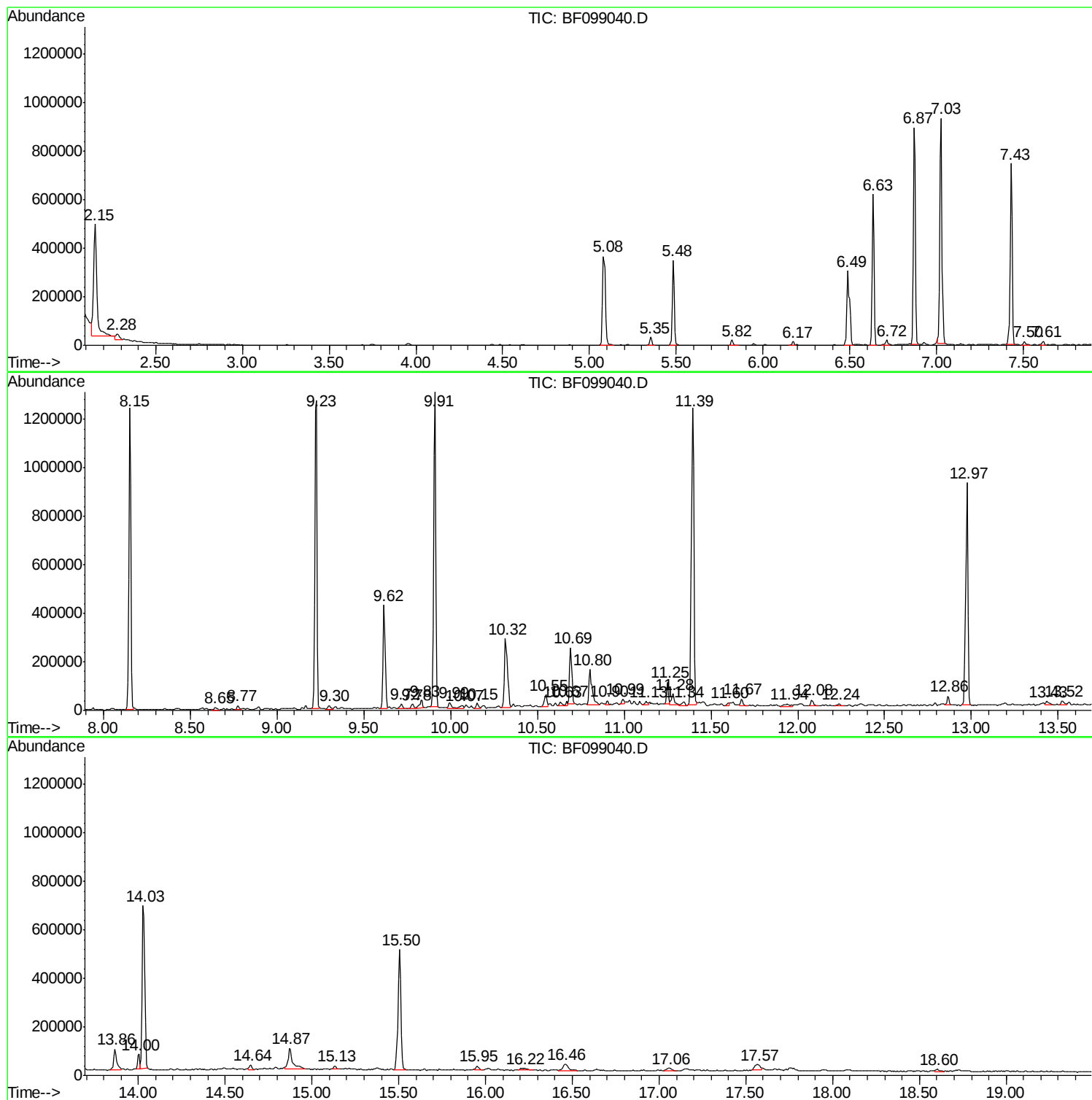
Sum of corrected areas: 13152463

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100317\
Data File : BF099040.D
Acq On : 3 Oct 2017 19:53
Operator : SJ/JU
Sample : I5496-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAMT-COMP-E

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100317\
Data File : BF099040.D
Acq On : 3 Oct 2017 19:53
Operator : SJ/JU
Sample : I5496-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAMT-COMP-E

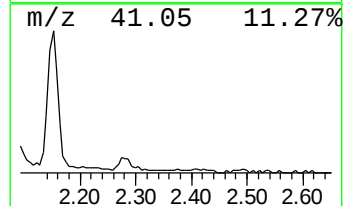
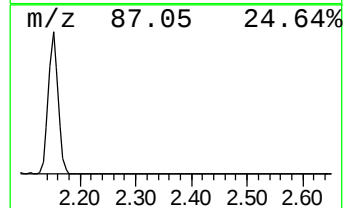
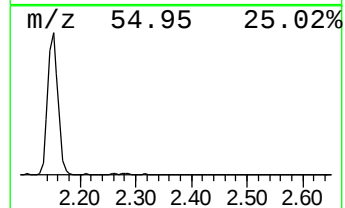
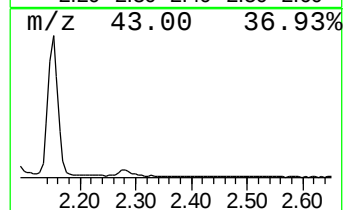
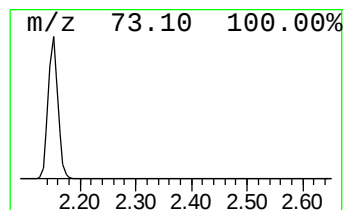
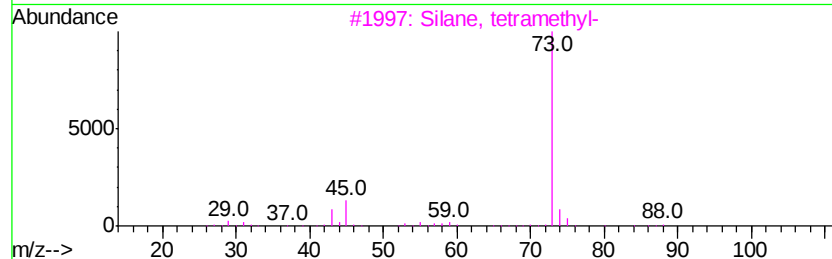
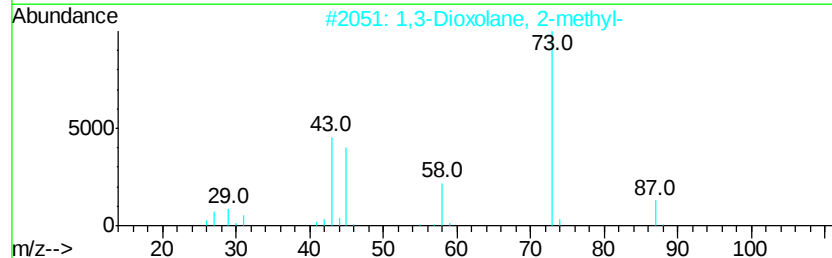
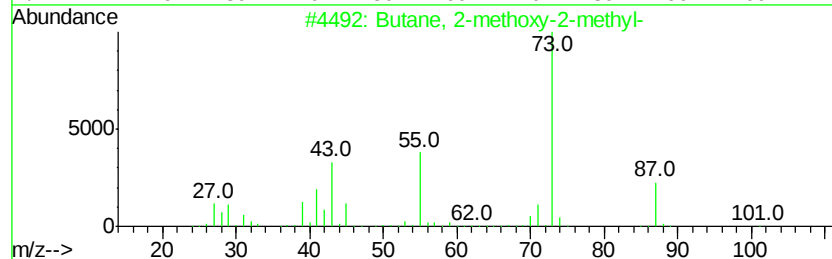
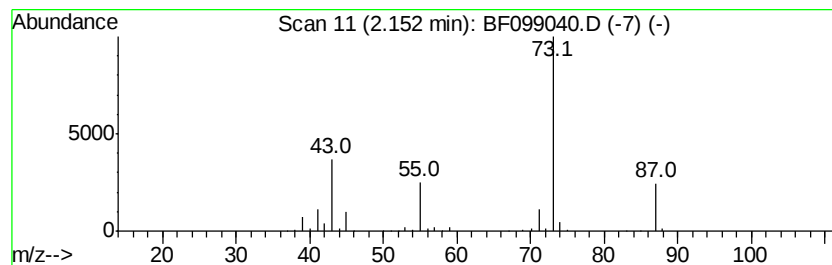
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.15	17.29 ng	673935	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5		Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100317\
Data File : BF099040.D
Acq On : 3 Oct 2017 19:53
Operator : SJ/JU
Sample : I5496-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAMT-COMP-E

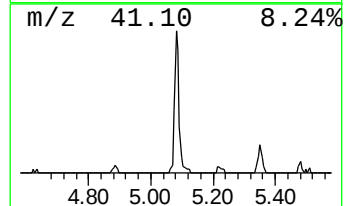
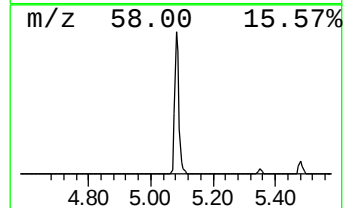
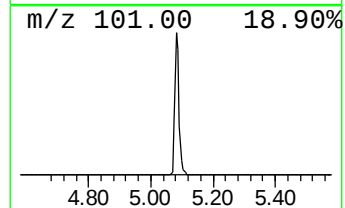
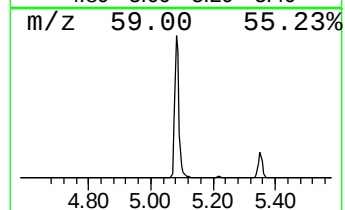
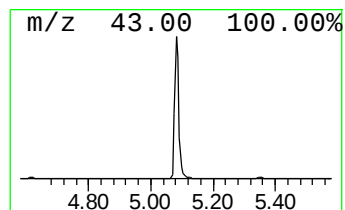
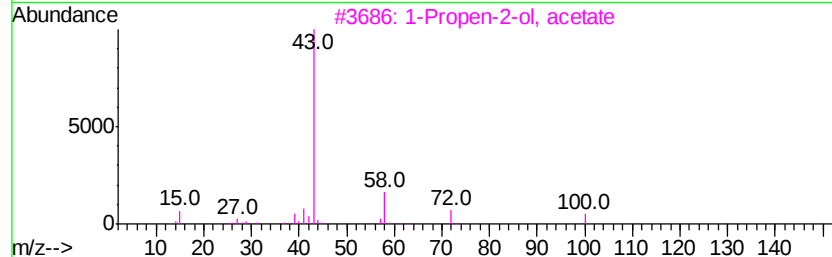
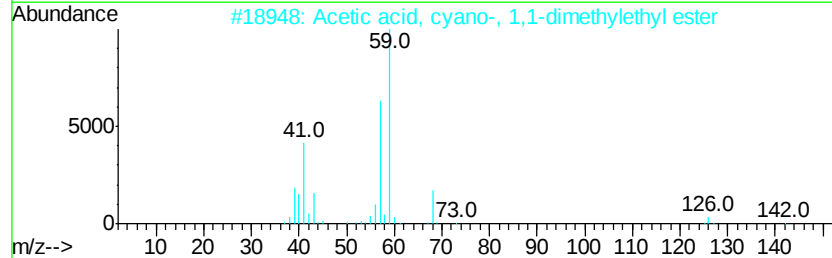
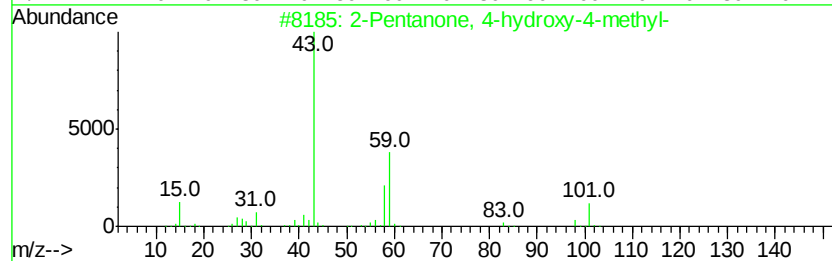
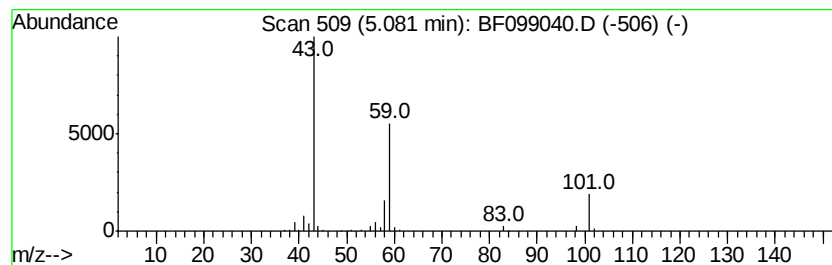
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	9.21 ng	358891	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100317\
Data File : BF099040.D
Acq On : 3 Oct 2017 19:53
Operator : SJ/JU
Sample : I5496-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAMT-COMP-E

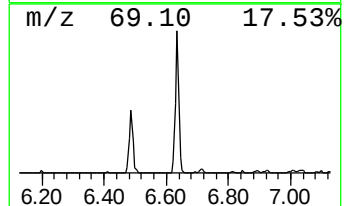
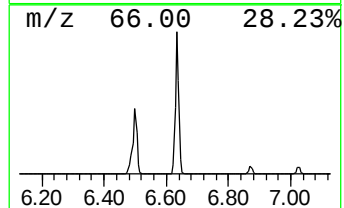
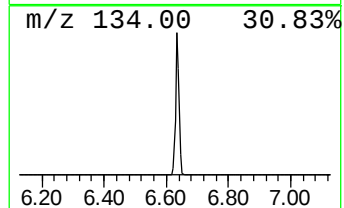
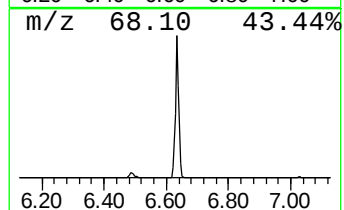
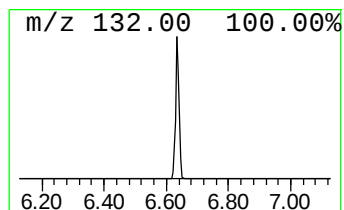
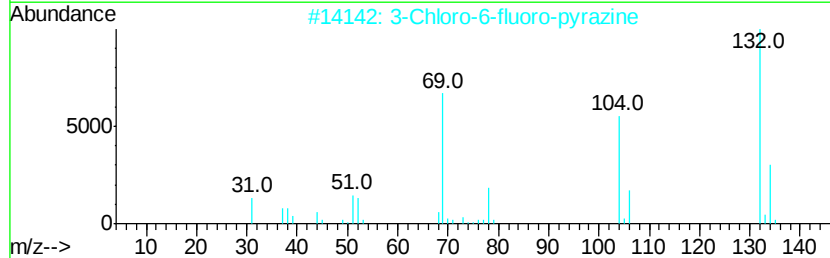
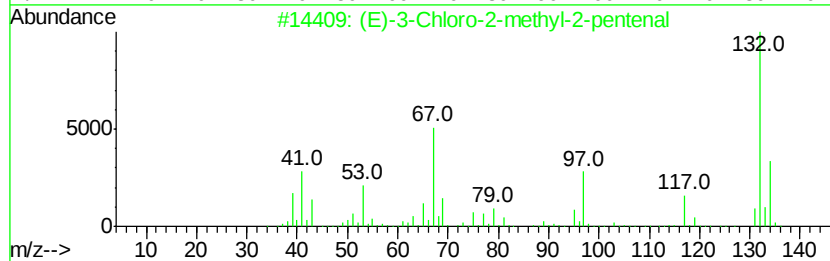
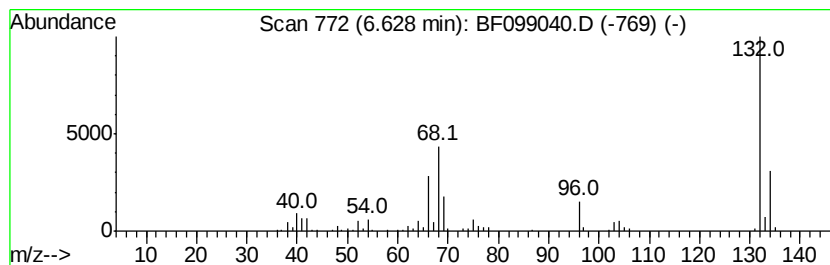
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.63 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	13.16 ng	512986	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100317\
Data File : BF099040.D
Acq On : 3 Oct 2017 19:53
Operator : SJ/JU
Sample : I5496-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAMT-COMP-E

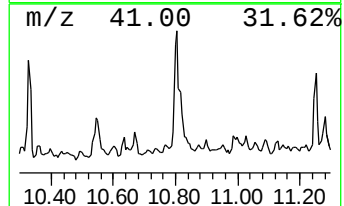
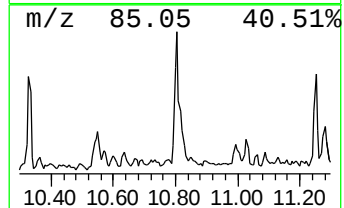
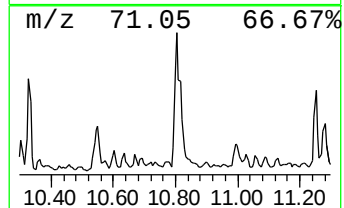
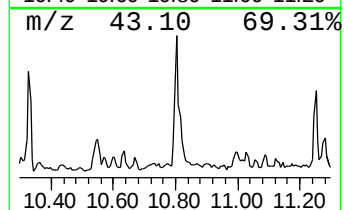
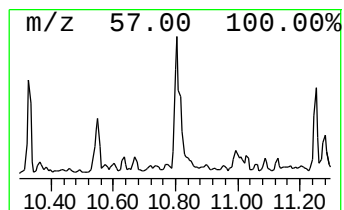
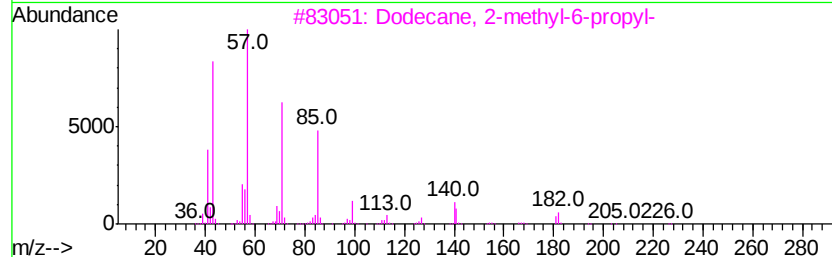
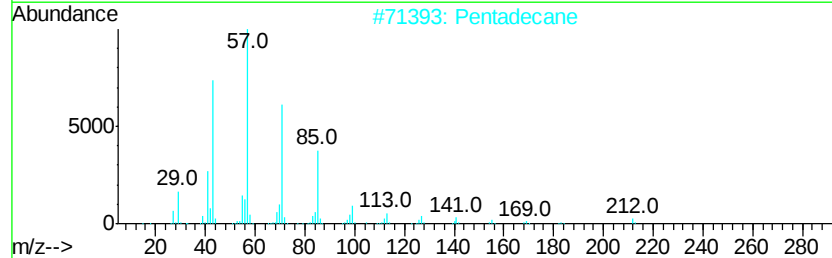
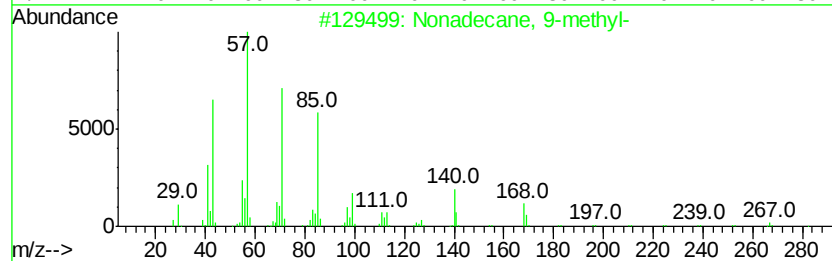
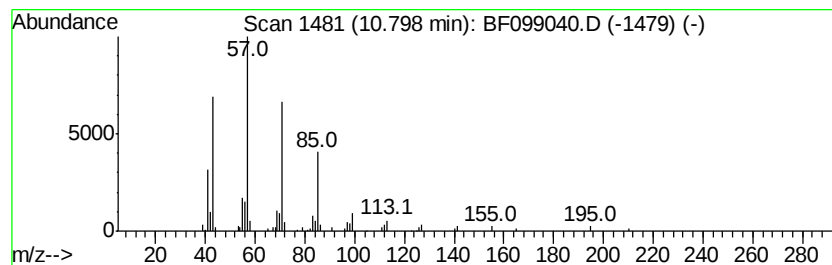
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Nonadecane, 9-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.80	3.44 ng	184036	Phenanthrene-d10	11.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	90
2		Pentadecane	212	C15H32	000629-62-9	87
3		Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	86
4		Tetradecane	198	C14H30	000629-59-4	86
5		Hexadecane	226	C16H34	000544-76-3	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100317\
Data File : BF099040.D
Acq On : 3 Oct 2017 19:53
Operator : SJ/JU
Sample : I5496-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

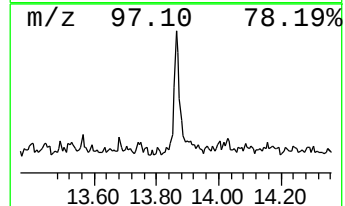
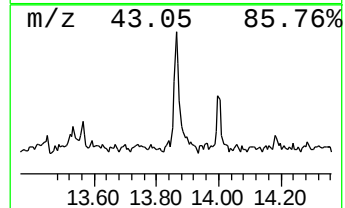
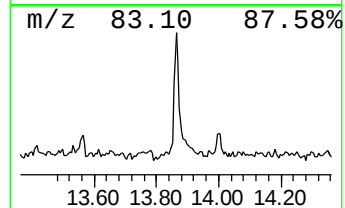
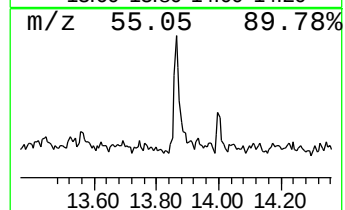
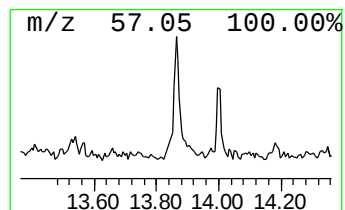
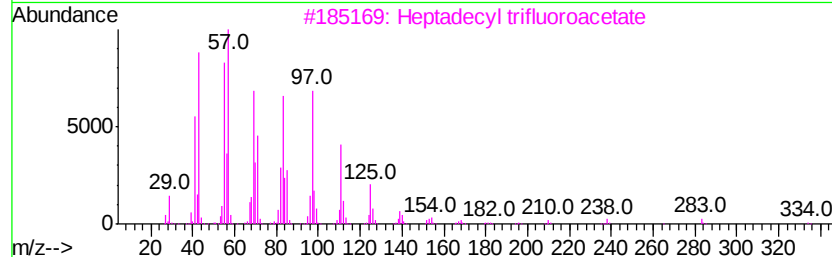
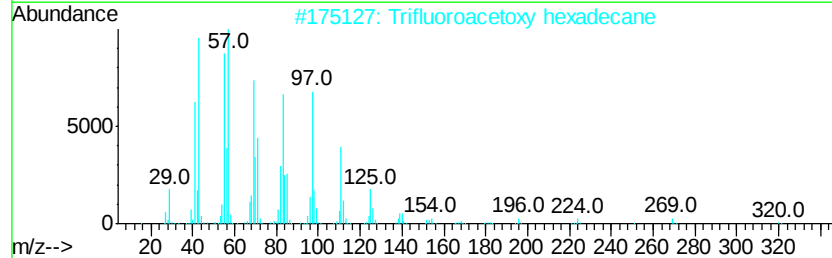
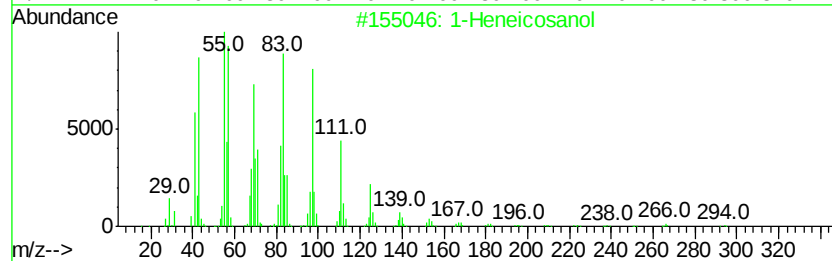
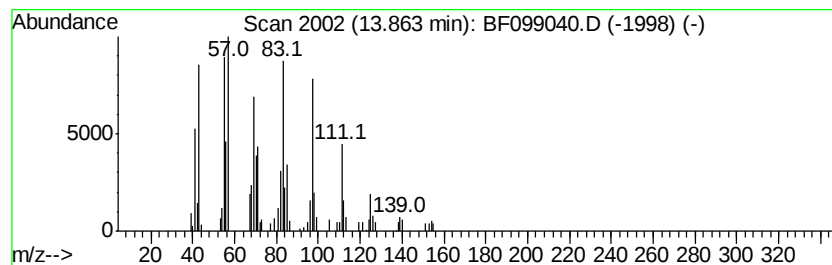
Instrument :
BNA_F
ClientSampleId :
PAMT-COMP-E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Heneicosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	3.40 ng	107664	Chrysene-d12	14.03
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Heneicosanol	312 C21H44O	015594-90-8	95
2	Trifluoroacetoxy hexadecane	338 C18H33F3O2	006222-03-3	95
3	Heptadecyl trifluoroacetate	352 C19H35F3O2	1000351-87-0	94
4	Octacosanol	410 C28H58O	000557-61-9	93
5	1-Nonadecene	266 C19H38	018435-45-5	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100317\
Data File : BF099040.D
Acq On : 3 Oct 2017 19:53
Operator : SJ/JU
Sample : I5496-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAMT-COMP-E

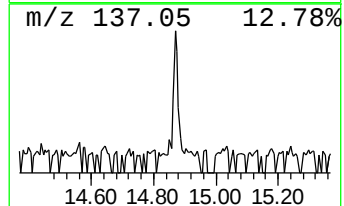
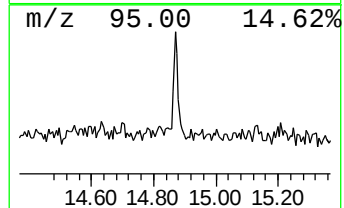
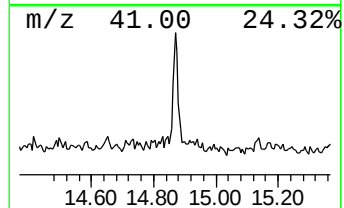
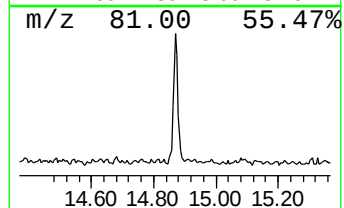
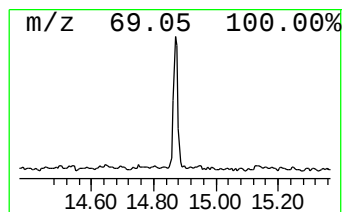
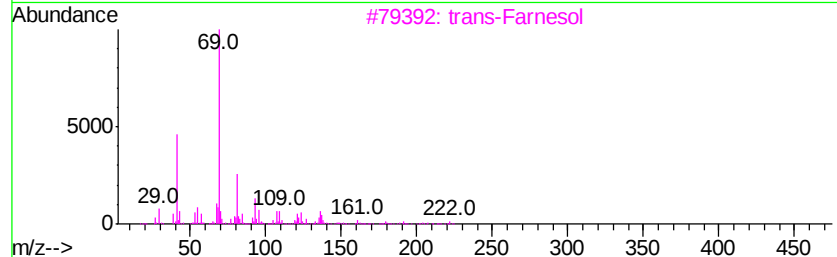
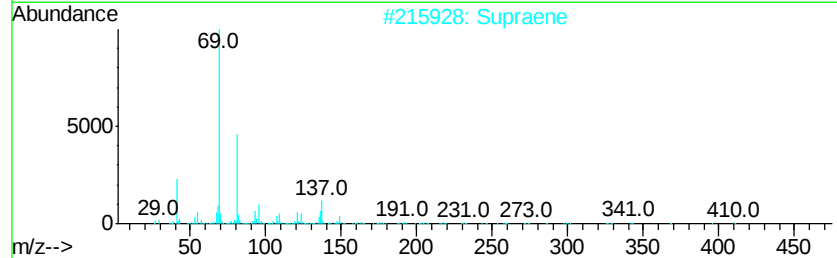
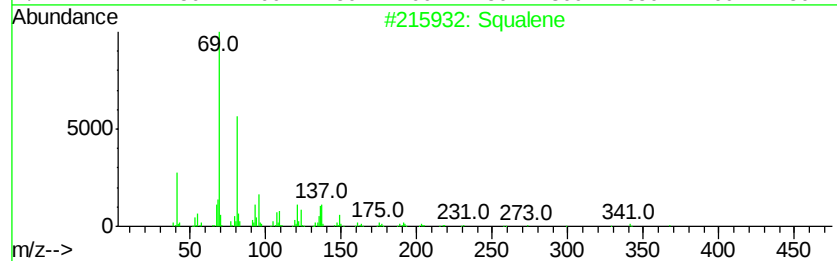
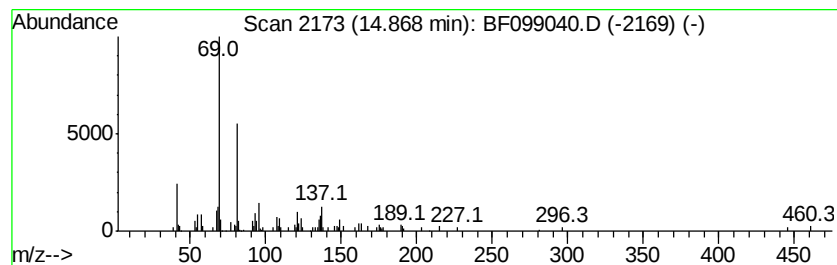
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	5.77 ng	167121	Perylene-d12	15.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	87
2		Supraene	410	C30H50	007683-64-9	83
3		trans-Farnesol	222	C15H26O	000106-28-5	53
4		1,5-Heptadiene, 3,4-dimethyl-	124	C9H16	1000061-77-9	50
5		Pentane, 1,4-dibromo-	228	C5H10Br2	000626-87-9	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100317\
Data File : BF099040.D
Acq On : 3 Oct 2017 19:53
Operator : SJ/JU
Sample : I5496-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAMT-COMP-E

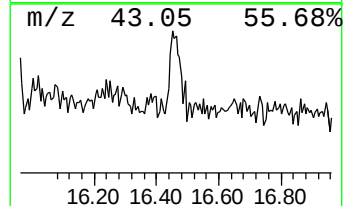
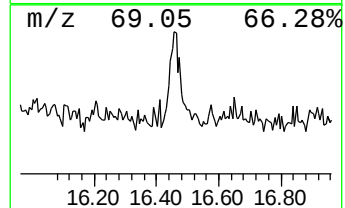
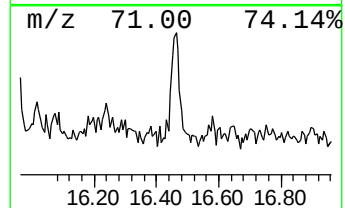
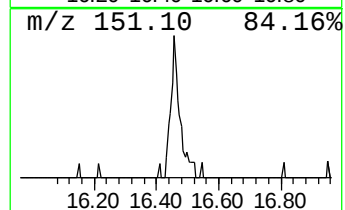
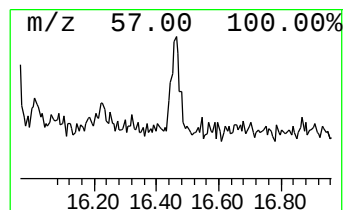
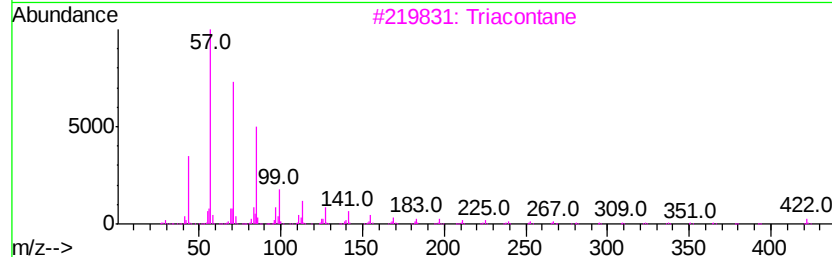
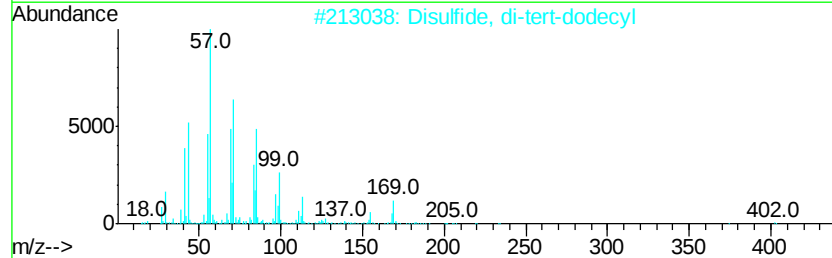
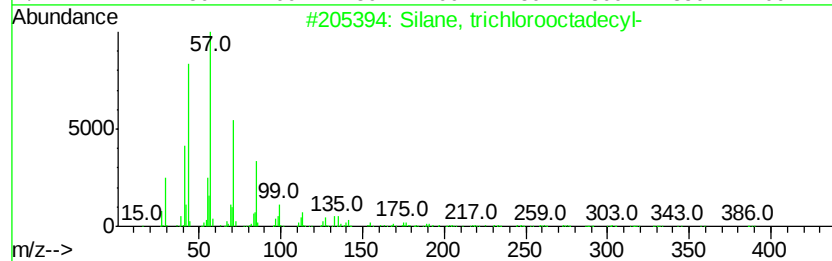
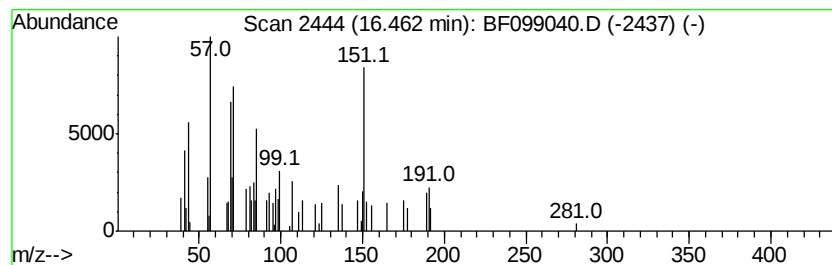
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown16.46 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.46	2.28 ng	65957	Perylene-d12	15.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	27
2		Disulfide, di-tert-dodecyl	402	C24H50S2	027458-90-8	25
3		Triacontane	422	C30H62	000638-68-6	22
4		Heneicosane	296	C21H44	000629-94-7	22
5		2-methyloctacosane	408	C29H60	1000376-72-8	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100317\
Data File : BF099040.D
Acq On : 3 Oct 2017 19:53
Operator : SJ/JU
Sample : I5496-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAMT-COMP-E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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
Butane, 2-methoxy...	2.15	17.3	ng	673935	1	6.87	779584	20.0
2-Pentanone, 4-hy...	5.08	9.2	ng	358891	1	6.87	779584	20.0
unknown6.63	6.63	13.2	ng	512986	1	6.87	779584	20.0
Nonadecane, 9-met...	10.80	3.4	ng	184036	4	11.39	1069530	20.0
1-Heneicosanol	13.86	3.4	ng	107664	5	14.03	634248	20.0
Squalene	14.87	5.8	ng	167121	6	15.50	579386	20.0
unknown16.46	16.46	2.3	ng	65957	6	15.50	579386	20.0