

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100417\
 Data File : BF099067.D
 Acq On : 4 Oct 2017 15:24
 Operator : SJ/JU
 Sample : I5584-01
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-1-COMP

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	2.163	9	13	30	rVB	244022	466711	7.78%	0.769%
2	5.098	507	512	526	rVB	521153	787572	13.12%	1.297%
3	5.493	573	579	582	rBV	3456907	3899444	64.97%	6.422%
4	6.504	738	751	754	rBV	3090178	4050134	67.49%	6.670%
5	6.640	768	774	777	rBV	3659096	3990439	66.49%	6.572%
6	6.863	807	812	816	rBV	1170401	1006174	16.77%	1.657%
7	7.022	835	839	842	rVB	3150279	3082066	51.35%	5.076%
8	7.434	903	909	912	rBV	2314179	2598551	43.30%	4.279%
9	7.516	917	923	934	rVB2	51817	80673	1.34%	0.133%
10	8.145	1026	1030	1033	rBV	1491816	1294439	21.57%	2.132%
11	9.222	1207	1213	1216	rBV	4077348	4316486	71.92%	7.109%
12	9.610	1276	1279	1283	rVB	825758	749442	12.49%	1.234%
13	9.692	1287	1293	1302	rVB3	113525	177273	2.95%	0.292%
14	9.904	1324	1329	1332	rBV	1490848	1448509	24.14%	2.385%
15	9.933	1332	1334	1337	rVB	213808	151455	2.52%	0.249%
16	10.104	1357	1363	1367	rBV2	110634	134264	2.24%	0.221%
17	10.298	1392	1396	1398	rBV2	50112	69019	1.15%	0.114%
18	10.322	1398	1400	1403	rVB	118715	98264	1.64%	0.162%
19	10.445	1418	1421	1424	rBV	203176	163905	2.73%	0.270%
20	10.692	1455	1463	1467	rBV	2342332	2783850	46.39%	4.585%
21	10.798	1477	1481	1487	rBV	120296	170312	2.84%	0.280%
22	11.245	1552	1557	1559	rBV2	101895	106711	1.78%	0.176%
23	11.280	1559	1563	1569	rVB2	114007	145041	2.42%	0.239%
24	11.386	1577	1581	1583	rBV	1501305	1475534	24.59%	2.430%
25	11.410	1583	1585	1589	rVV	1331537	1168986	19.48%	1.925%
26	11.463	1589	1594	1597	rVB	486404	412150	6.87%	0.679%
27	11.604	1613	1618	1626	rBV2	113175	182373	3.04%	0.300%
28	11.669	1626	1629	1635	rVB2	58052	69717	1.16%	0.115%
29	11.886	1663	1666	1668	rBV	102331	105147	1.75%	0.173%
30	11.910	1668	1670	1674	rVV2	322229	290175	4.84%	0.478%
31	11.998	1682	1685	1688	rBV	267647	291110	4.85%	0.479%
32	12.139	1690	1709	1719	rBV2	1231613	6001500	100.00%	9.884%
33	12.474	1754	1766	1773	rBV	683702	1755534	29.25%	2.891%
34	12.604	1783	1788	1791	rBV	2029194	1800075	29.99%	2.964%

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100417\
 Data File : BF099067.D
 Acq On : 4 Oct 2017 15:24
 Operator : SJ/JU
 Sample : I5584-01
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-1-COMP

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	12.692	1800	1803	1805	rBV2	66318	69416	1.16%	0.114%
36	12.833	1820	1827	1830	rBV	1528759	1694138	28.23%	2.790%
37	12.974	1843	1851	1855	rBV	3427968	3967782	66.11%	6.534%
38	13.045	1858	1863	1866	rBV2	52997	89720	1.49%	0.148%
39	13.133	1874	1878	1879	rBV3	52556	63226	1.05%	0.104%
40	13.157	1879	1882	1886	rVV	174964	173156	2.89%	0.285%
41	13.221	1890	1893	1895	rBV	171415	155560	2.59%	0.256%
42	13.257	1895	1899	1903	rVB2	130317	201199	3.35%	0.331%
43	13.657	1965	1967	1973	rVB3	69344	84370	1.41%	0.139%
44	13.774	1984	1987	1989	rBV	90718	76470	1.27%	0.126%
45	13.851	1997	2000	2011	rVB3	393499	521804	8.69%	0.859%
46	13.974	2012	2021	2025	rBV7	102682	322098	5.37%	0.530%
47	14.027	2025	2030	2032	rVV2	1434688	1832377	30.53%	3.018%
48	14.051	2032	2034	2042	rVB	639429	556576	9.27%	0.917%
49	14.133	2044	2048	2051	rVB	127487	117849	1.96%	0.194%
50	14.486	2104	2108	2113	rBV5	45997	97350	1.62%	0.160%
51	14.551	2113	2119	2123	rVV4	108663	200307	3.34%	0.330%
52	14.604	2123	2128	2141	rVB8	66234	188935	3.15%	0.311%
53	14.739	2146	2151	2156	rVV2	141032	251339	4.19%	0.414%
54	14.792	2156	2160	2171	rVB3	99571	210985	3.52%	0.347%
55	14.904	2173	2179	2194	rVB4	313111	691329	11.52%	1.139%
56	15.063	2202	2206	2209	rBV	344172	475662	7.93%	0.783%
57	15.092	2209	2211	2214	rVB	144306	138862	2.31%	0.229%
58	15.174	2222	2225	2228	rVB	65946	70182	1.17%	0.116%
59	15.274	2237	2242	2248	rBV7	46839	111297	1.85%	0.183%
60	15.368	2254	2258	2264	rBV	201322	262468	4.37%	0.432%
61	15.433	2265	2269	2274	rVB	286948	342880	5.71%	0.565%
62	15.498	2275	2280	2284	rBV	737354	949536	15.82%	1.564%
63	15.815	2329	2334	2339	rBV5	62174	113008	1.88%	0.186%
64	15.921	2345	2352	2361	rVB4	154976	390416	6.51%	0.643%
65	16.080	2373	2379	2386	rBV5	63524	157997	2.63%	0.260%
66	16.174	2390	2395	2401	rVB8	45014	91464	1.52%	0.151%
67	16.368	2422	2428	2435	rBV7	41533	89297	1.49%	0.147%
68	16.668	2476	2479	2489	rVB8	48430	102048	1.70%	0.168%
69	16.968	2524	2530	2537	rVB2	108672	211752	3.53%	0.349%
70	17.133	2553	2558	2565	rVB4	23372	61271	1.02%	0.101%
71	17.415	2600	2606	2610	rBV	86758	179538	2.99%	0.296%

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100417\
Data File : BF099067.D
Acq On : 4 Oct 2017 15:24
Operator : SJ/JU
Sample : I5584-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1-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-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	17.827	2669	2676	2677	rBV6	44378	85549	1.43%	0.141%
----	--------	------	------	------	------	-------	-------	-------	--------

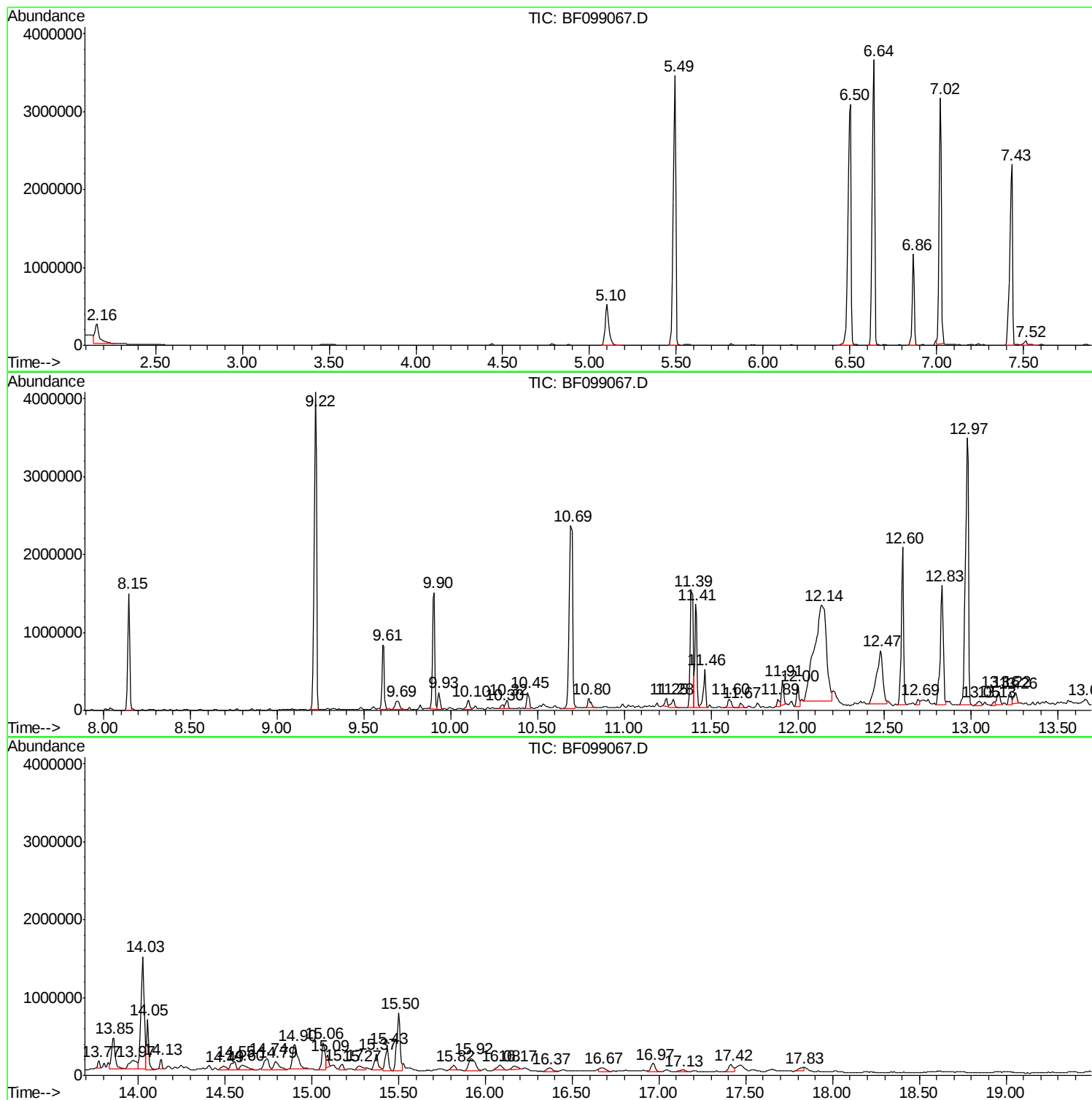
Sum of corrected areas: 60722248

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100417\
Data File : BF099067.D
Acq On : 4 Oct 2017 15:24
Operator : SJ/JU
Sample : I5584-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1-COMP

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\BF100417\
Data File : BF099067.D
Acq On : 4 Oct 2017 15:24
Operator : SJ/JU
Sample : I5584-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1-COMP

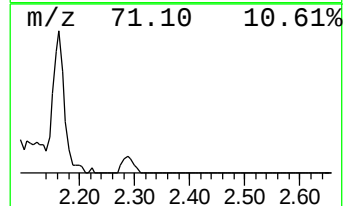
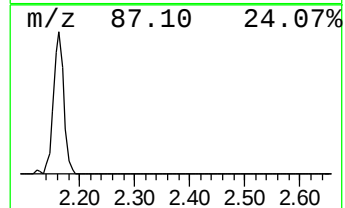
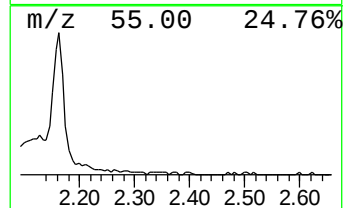
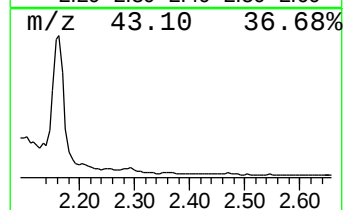
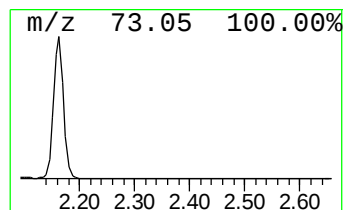
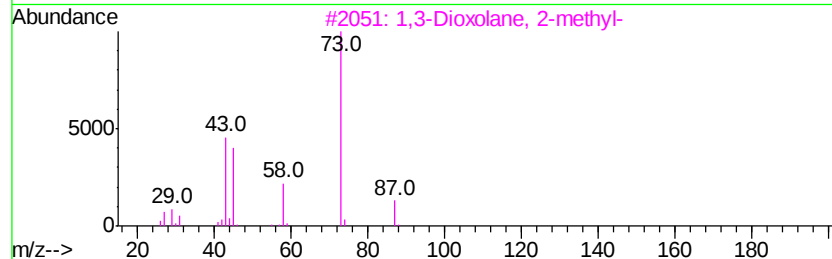
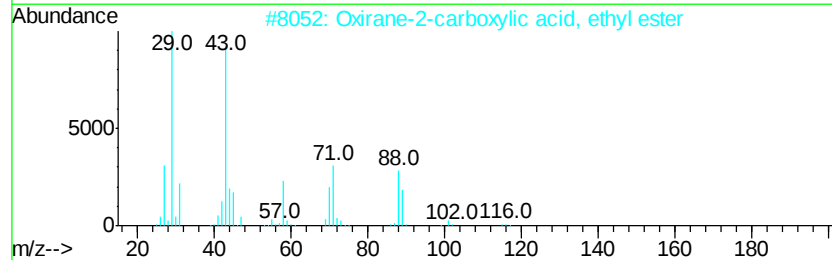
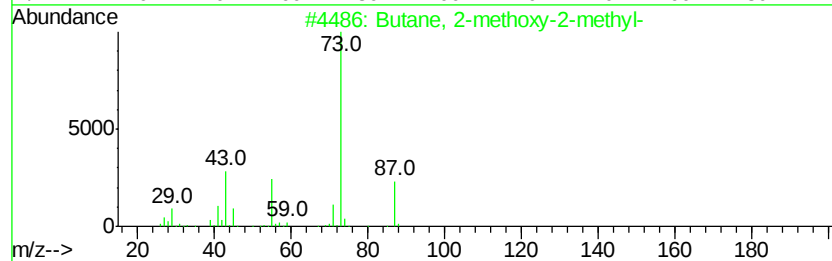
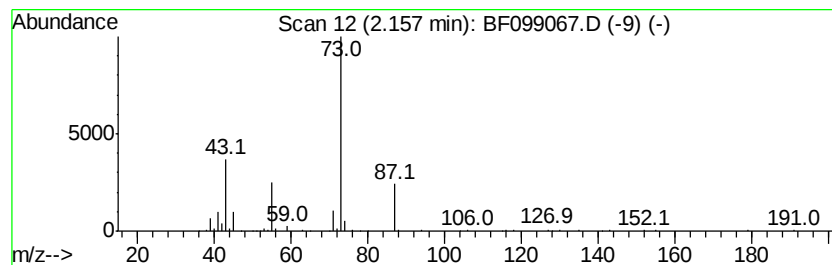
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	9.28 ng	466711	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		Oxirane-2-carboxylic acid, ethyl...	116	C5H8O3	1000192-50-3	9
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
4		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	9
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100417\
Data File : BF099067.D
Acq On : 4 Oct 2017 15:24
Operator : SJ/JU
Sample : I5584-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1-COMP

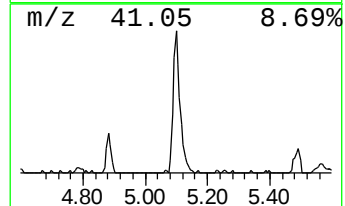
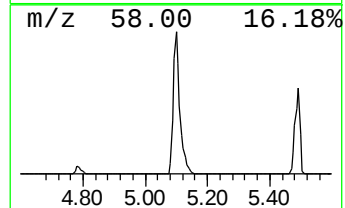
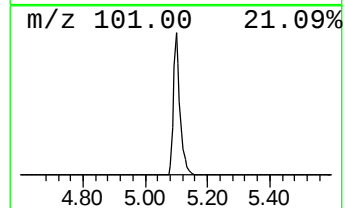
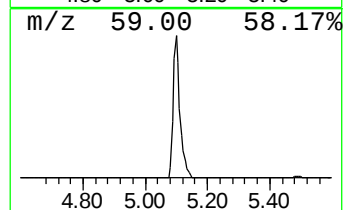
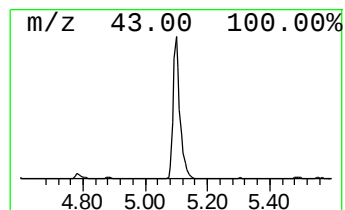
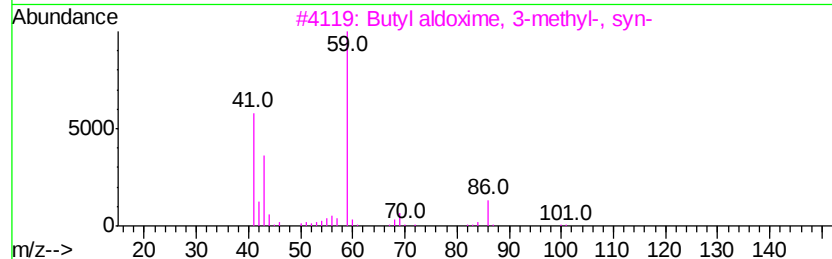
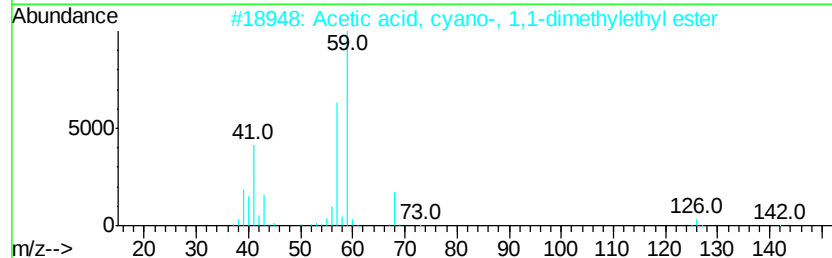
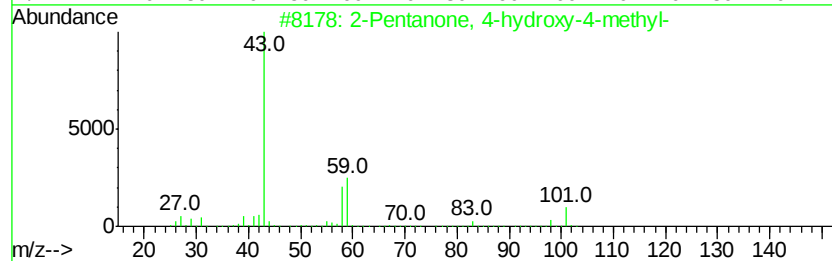
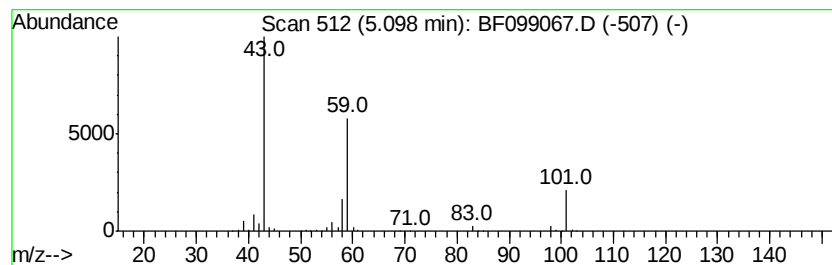
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	15.65 ng	787572	1,4-Dichlorobenzene-d4	6.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2		000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2		001116-98-9	23
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO		005780-40-5	9
4	Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4		006118-50-9	9
5	3-Hexanol, 4-methyl-	116	C7H16O		000615-29-2	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100417\
Data File : BF099067.D
Acq On : 4 Oct 2017 15:24
Operator : SJ/JU
Sample : I5584-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1-COMP

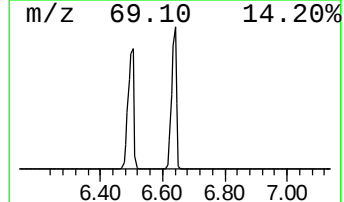
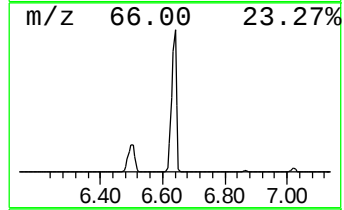
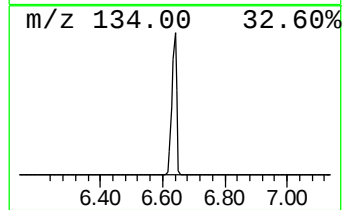
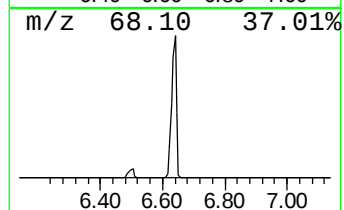
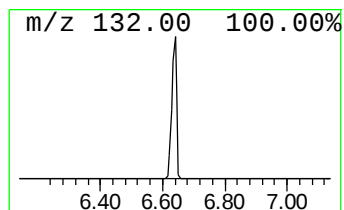
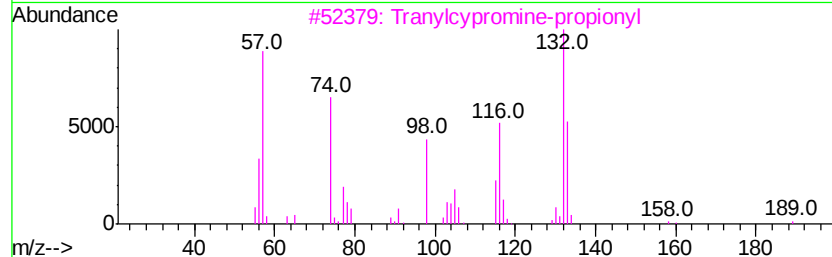
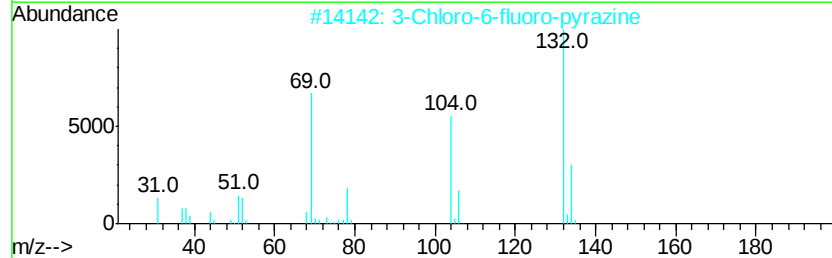
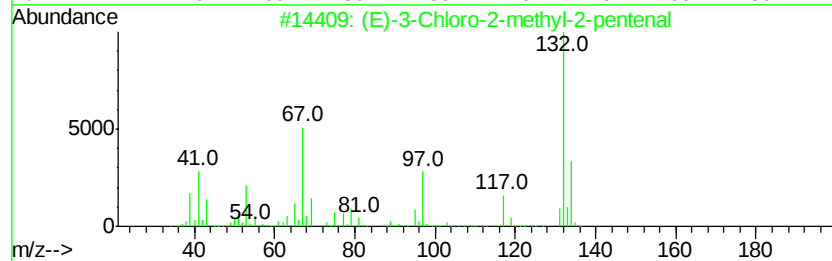
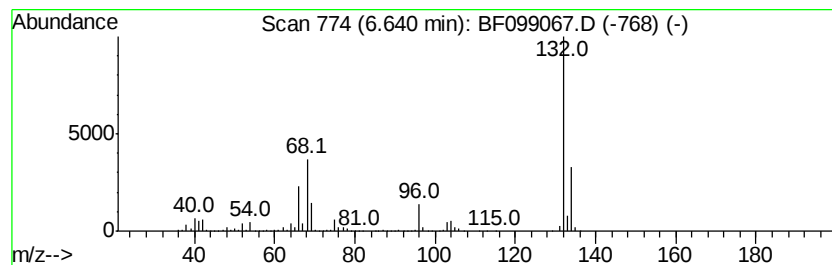
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.64 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	79.32 ng	3990440	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100417\
Data File : BF099067.D
Acq On : 4 Oct 2017 15:24
Operator : SJ/JU
Sample : I5584-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

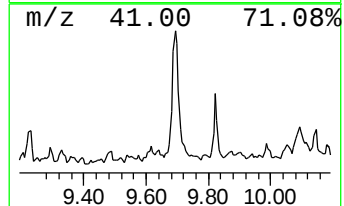
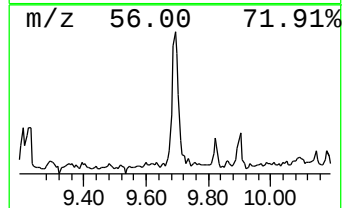
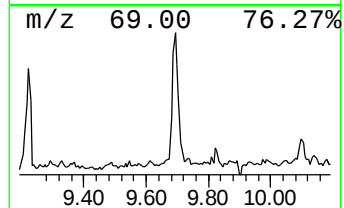
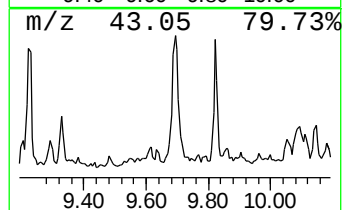
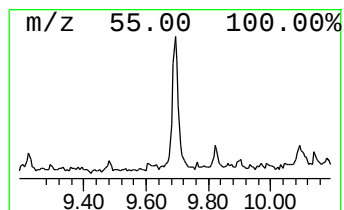
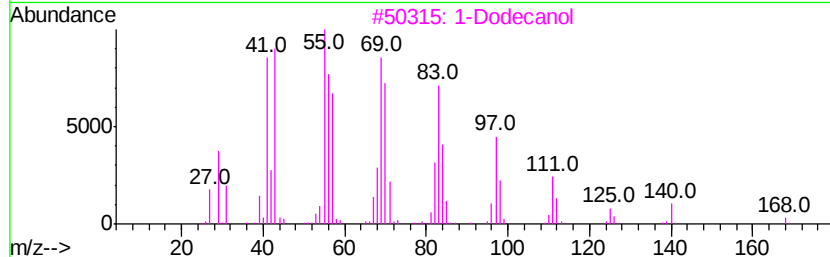
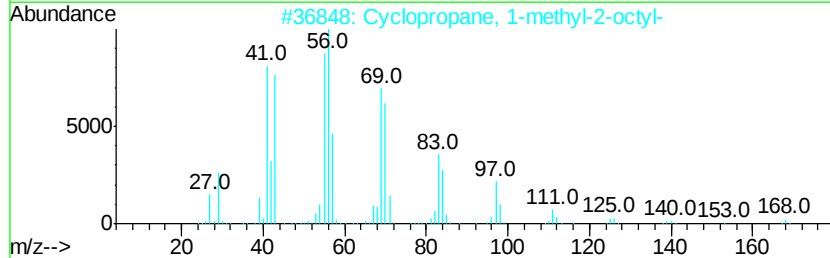
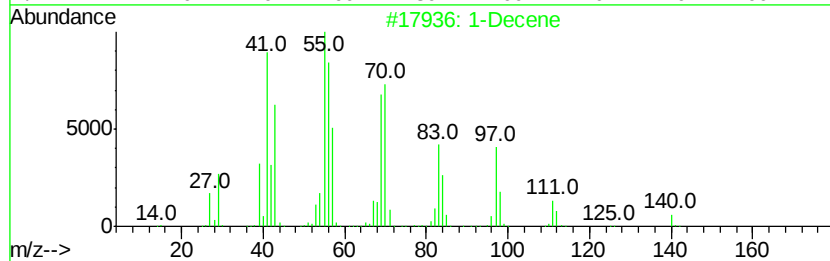
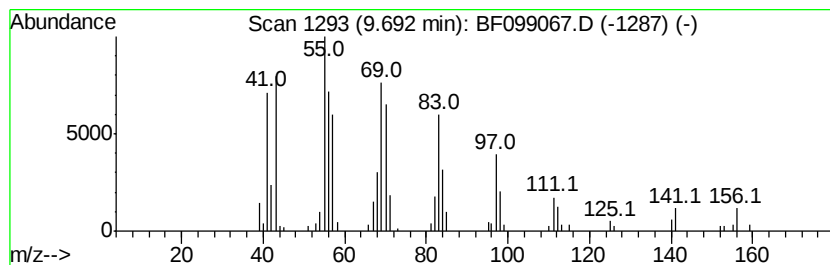
Instrument :
BNA_F
ClientSampleId :
TP-1-COMP

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 1-Decene Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.69	2.45 ng	177273	Acenaphthene-d10	9.90
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Decene		140 C10H20	000872-05-9 91
2	Cyclopropane, 1-methyl-2-octyl-		168 C12H24	037617-26-8 86
3	1-Dodecanol		186 C12H26O	000112-53-8 86
4	1-Undecanol		172 C11H24O	000112-42-5 86
5	Cyclodecane		140 C10H20	000293-96-9 83



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100417\
Data File : BF099067.D
Acq On : 4 Oct 2017 15:24
Operator : SJ/JU
Sample : I5584-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1-COMP

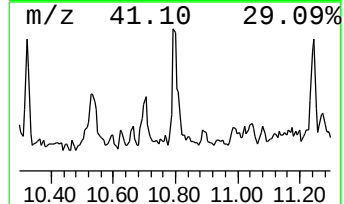
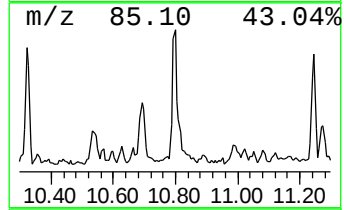
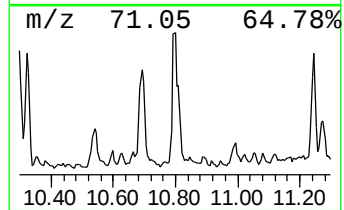
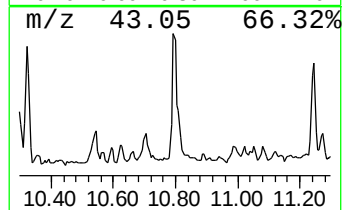
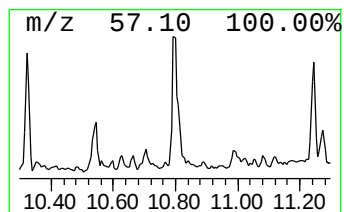
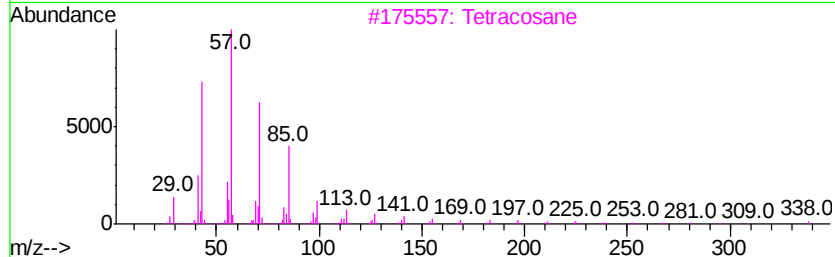
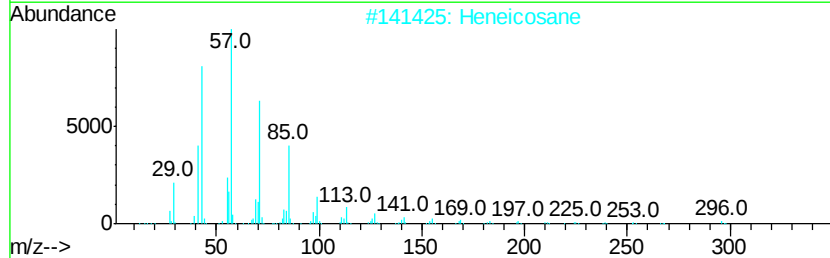
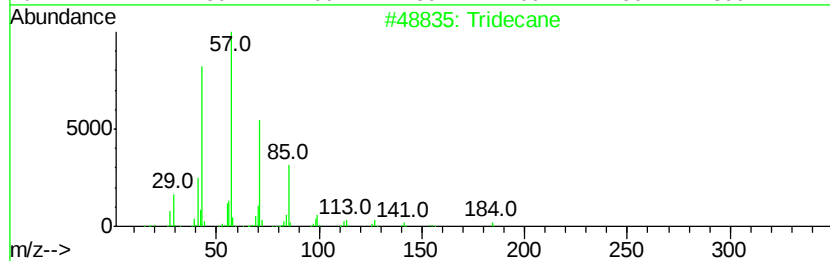
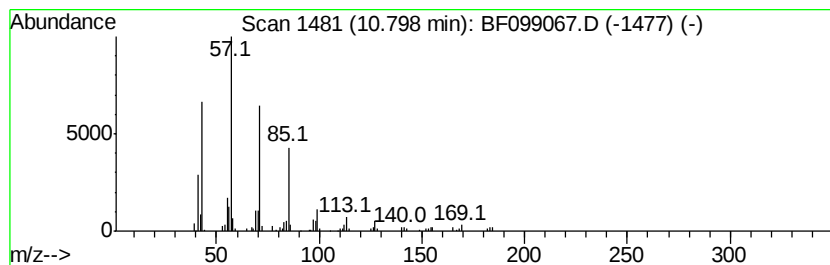
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Tridecane Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.80	2.31 ng	170312	Phenanthrene-d10	11.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tridecane	184	C13H28	000629-50-5	94
2		Heneicosane	296	C21H44	000629-94-7	91
3		Tetracosane	338	C24H50	000646-31-1	91
4		Hexadecane	226	C16H34	000544-76-3	90
5		Octadecane	254	C18H38	000593-45-3	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100417\
Data File : BF099067.D
Acq On : 4 Oct 2017 15:24
Operator : SJ/JU
Sample : I5584-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1-COMP

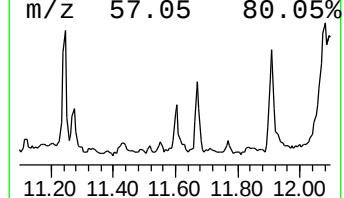
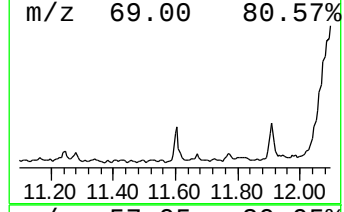
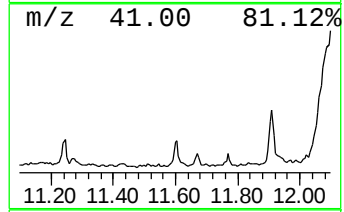
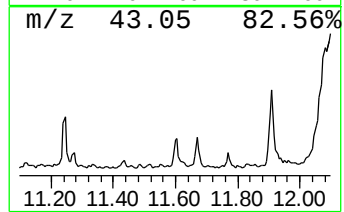
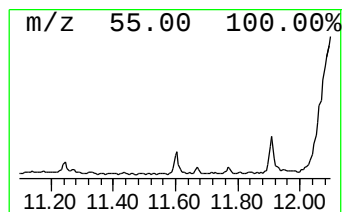
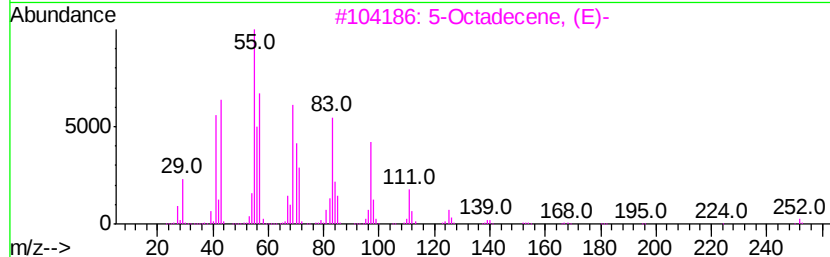
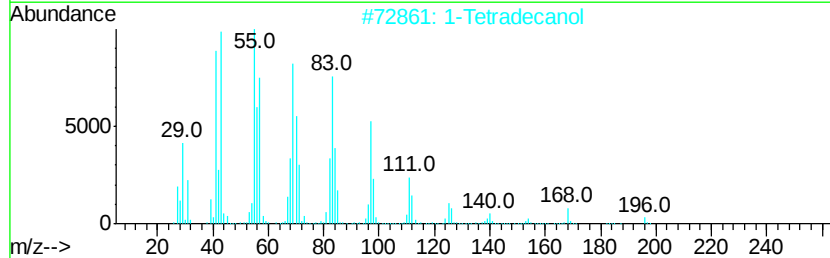
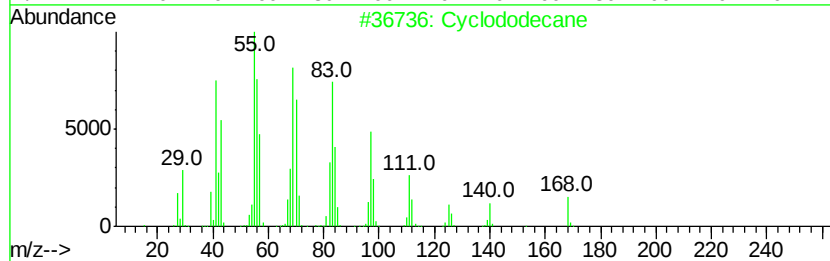
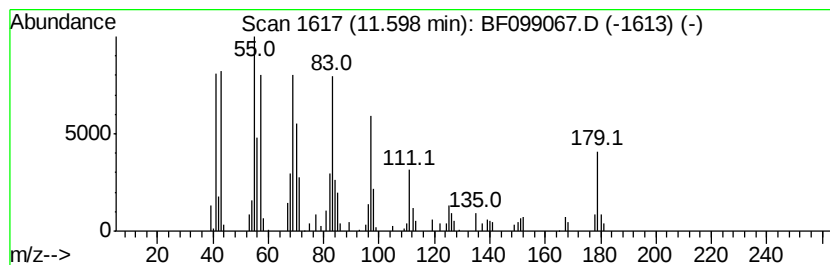
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cyclododecane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.60	2.47 ng	182373	Phenanthrene-d10	11.39

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclododecane	168	C12H24	000294-62-2	94
2		1-Tetradecanol	214	C14H30O	000112-72-1	87
3		5-Octadecene, (E)-	252	C18H36	007206-21-5	87
4		1-Hexadecanol	242	C16H34O	036653-82-4	87
5		Dichloroacetic acid, tridecyl ester	310	C15H28Cl2O2	1000280-48-3	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100417\
Data File : BF099067.D
Acq On : 4 Oct 2017 15:24
Operator : SJ/JU
Sample : I5584-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1-COMP

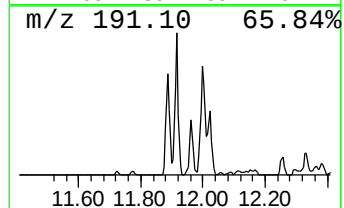
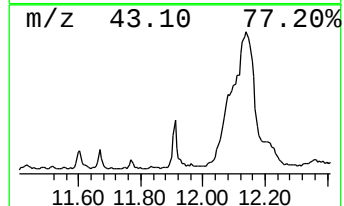
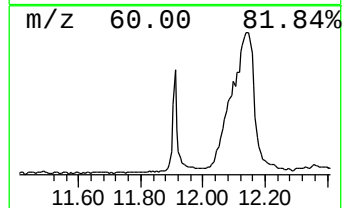
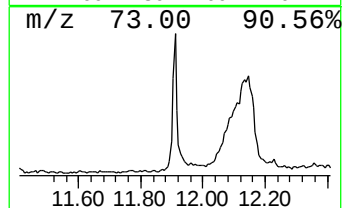
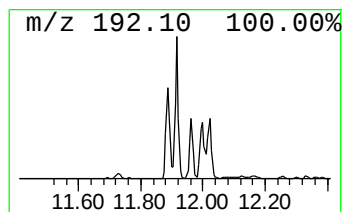
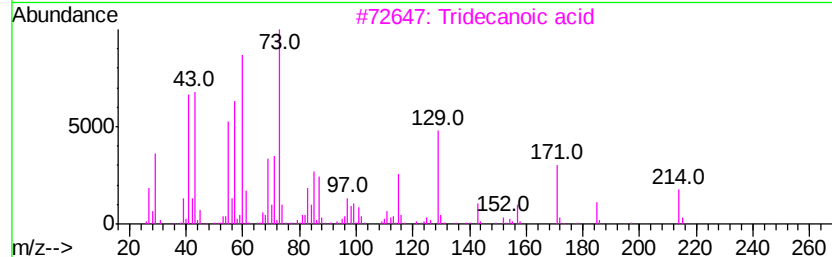
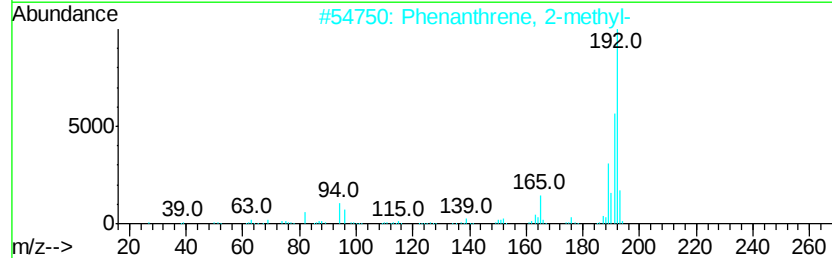
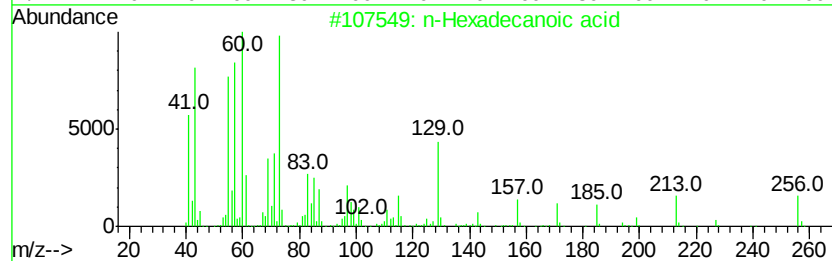
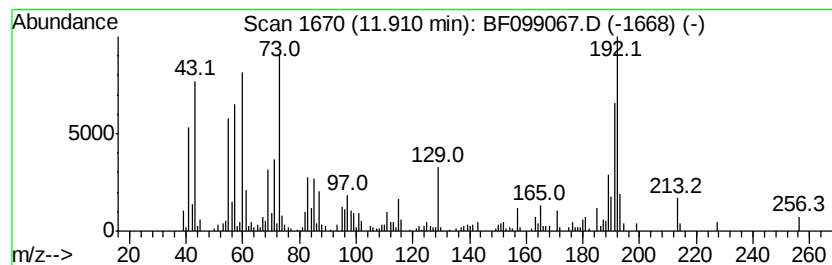
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Hexadecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.91	3.93 ng	290175	Phenanthrene-d10	11.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2		Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	93
3		Tridecanoic acid	214	C13H26O2	000638-53-9	86
4		Anthracene, 2-methyl-	192	C15H12	000613-12-7	86
5		Anthracene, 1-methyl-	192	C15H12	000610-48-0	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100417\
Data File : BF099067.D
Acq On : 4 Oct 2017 15:24
Operator : SJ/JU
Sample : I5584-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

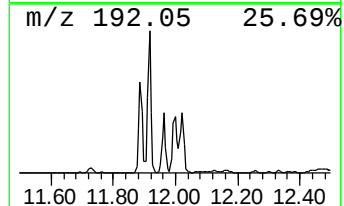
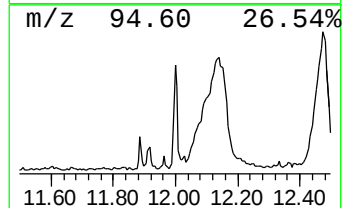
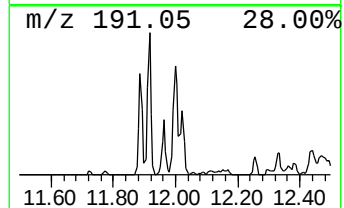
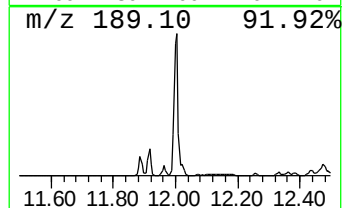
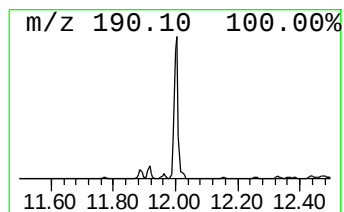
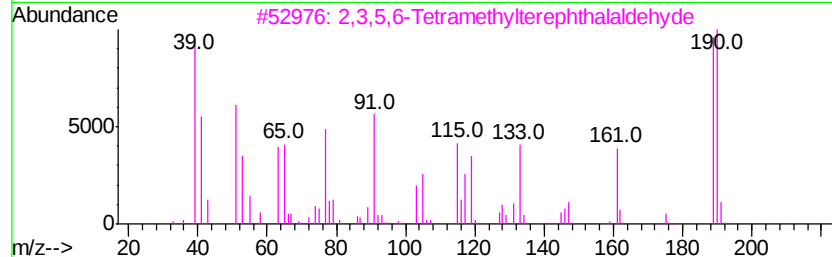
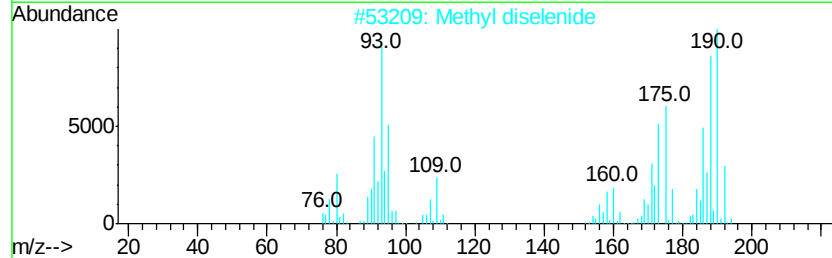
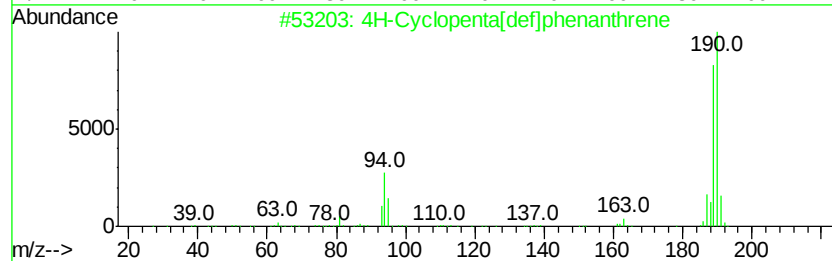
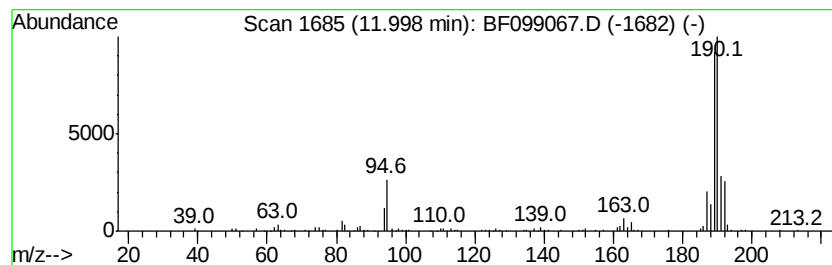
Instrument :
BNA_F
ClientSampleId :
TP-1-COMP

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 9 4H-Cyclopenta[def]phenanthrene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.00	3.95 ng	291110	Phenanthrene-d10	11.39	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	94
2	Methyl diselenide	190	C2H6Se2	007101-31-7	45
3	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	43
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	38
5	1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	16



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100417\
Data File : BF099067.D
Acq On : 4 Oct 2017 15:24
Operator : SJ/JU
Sample : I5584-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1-COMP

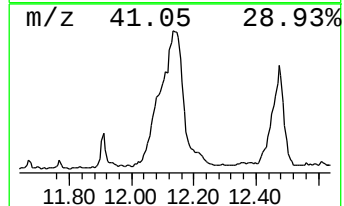
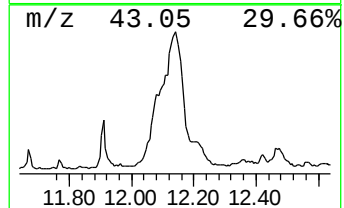
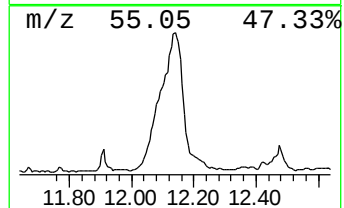
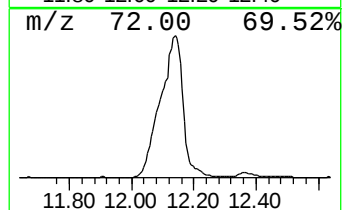
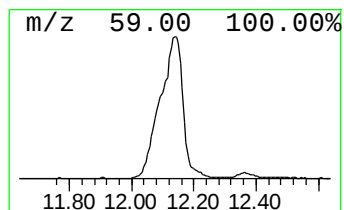
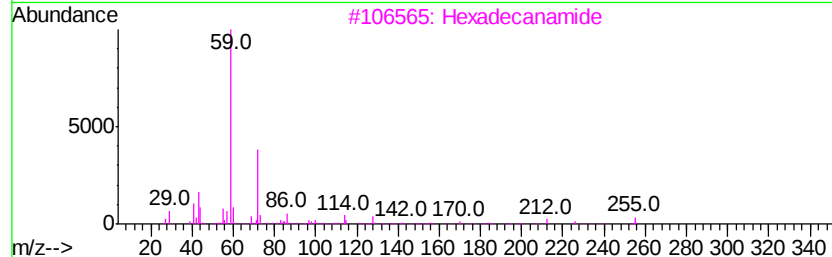
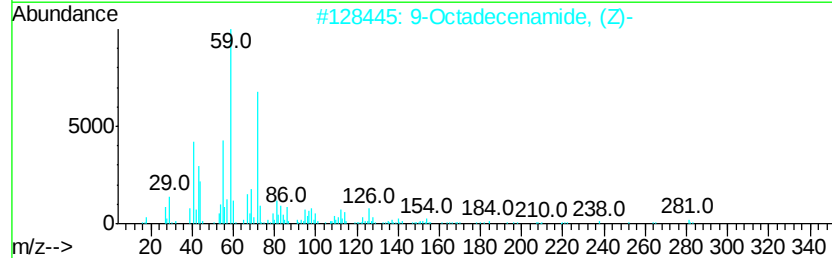
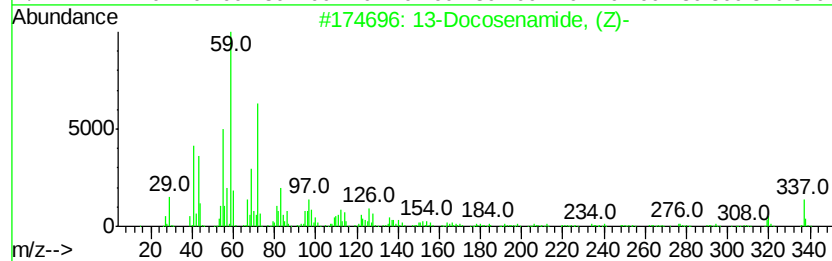
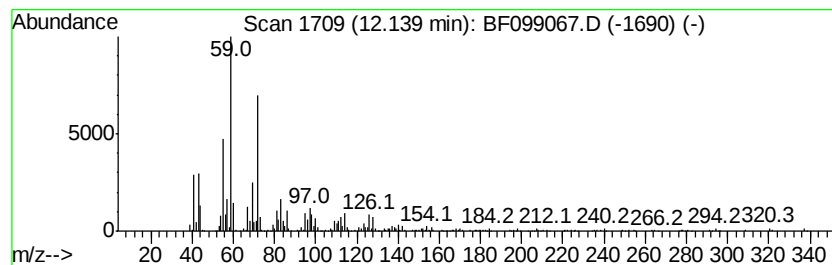
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 13-Docosenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.14	81.35 ng	6001500	Phenanthrene-d10	11.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	91
2		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
3		Hexadecanamide	255	C16H33NO	000629-54-9	72
4		Tetradecanamide	227	C14H29NO	000638-58-4	59
5		Decanamide-	171	C10H21NO	002319-29-1	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100417\
Data File : BF099067.D
Acq On : 4 Oct 2017 15:24
Operator : SJ/JU
Sample : I5584-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1-COMP

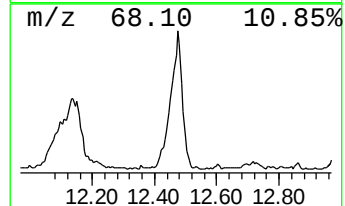
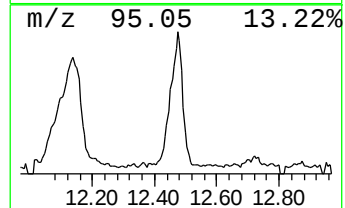
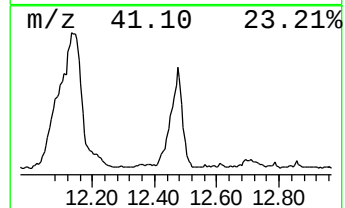
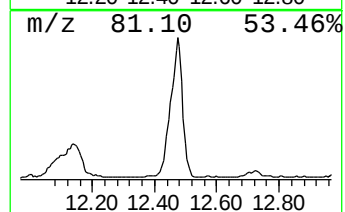
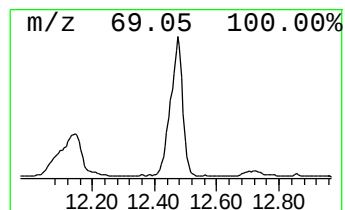
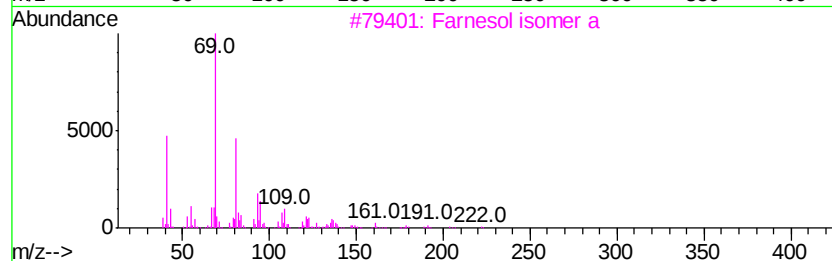
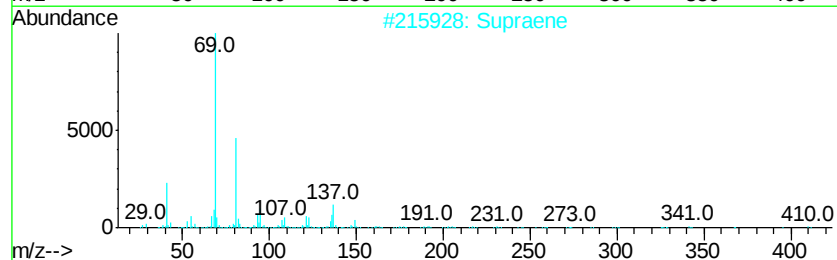
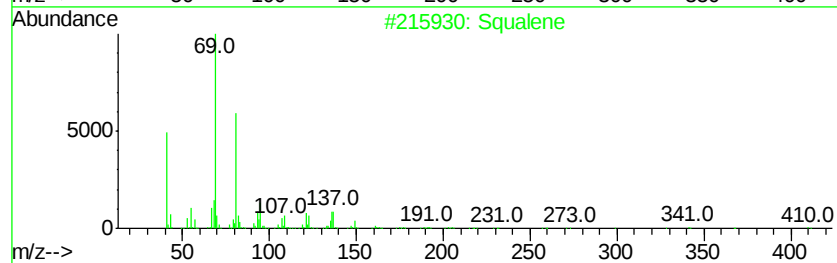
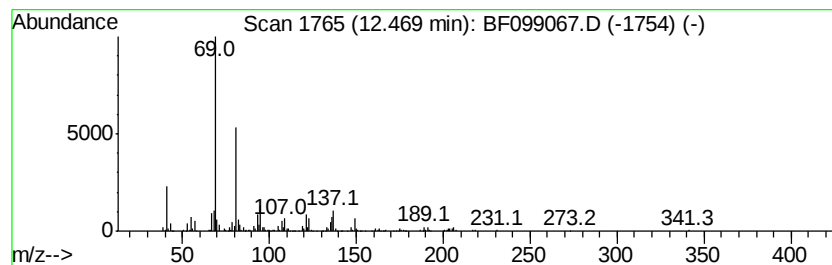
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.47	23.80 ng	1755530	Phenanthrene-d10	11.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	91
3		Farnesol isomer a	222	C15H26O	1000108-92-4	74
4		2,6-Octadiene, 4-methyl-	124	C9H16	074498-94-5	50
5		2,6-Octadiene, 4,5-dimethyl-	138	C10H18	018476-57-8	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100417\
Data File : BF099067.D
Acq On : 4 Oct 2017 15:24
Operator : SJ/JU
Sample : I5584-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

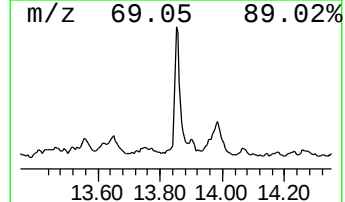
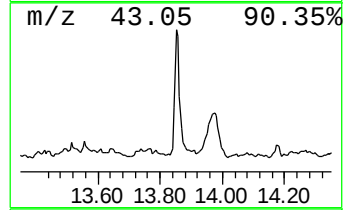
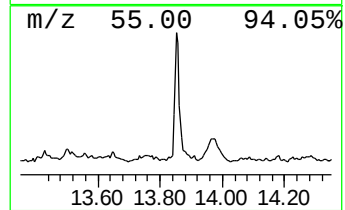
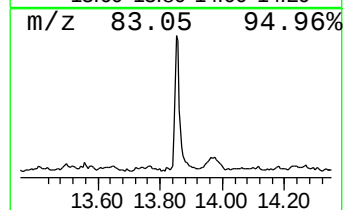
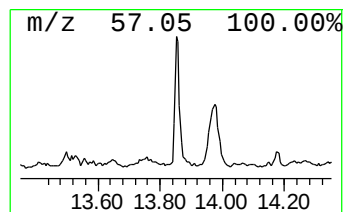
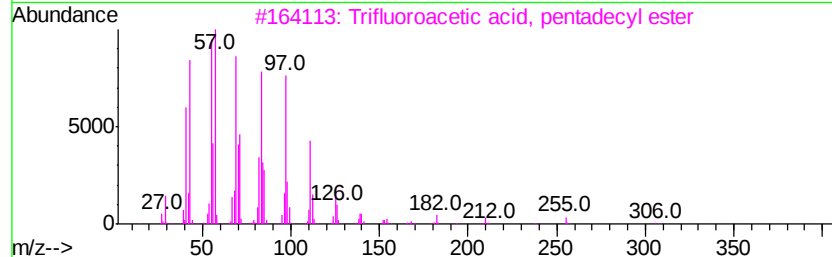
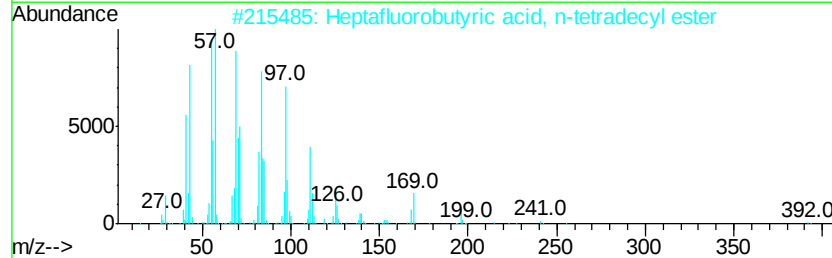
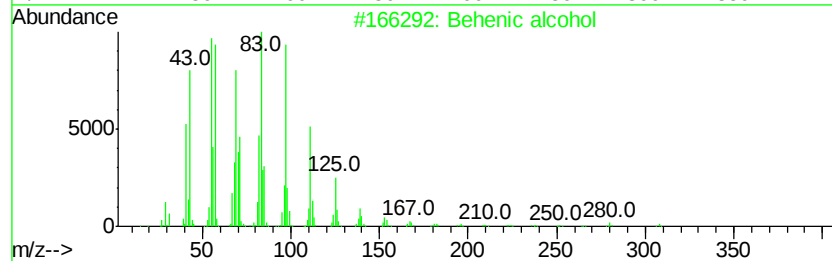
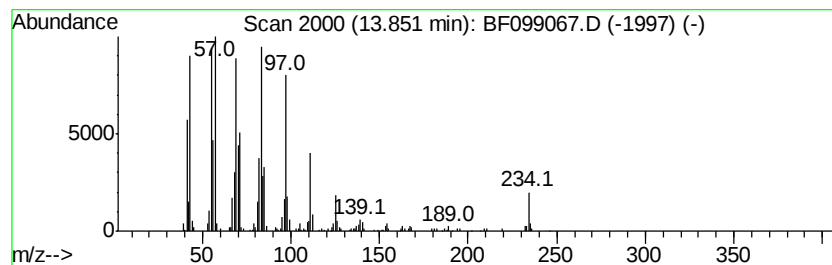
Instrument :
BNA_F
ClientSampleId :
TP-1-COMP

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 12 Behenic alcohol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	5.70 ng	521804	Chrysene-d12	14.03
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Behenic alcohol	326 C22H46O	000661-19-8 94
2		Heptafluorobutyric acid, n-tetra...	410 C18H29F7O2	007365-36-8 94
3		Trifluoroacetic acid, pentadecyl...	324 C17H31F3O2	959010-23-2 94
4		Trifluoroacetoxv hexadecane	338 C18H33F3O2	006222-03-3 94
5		Pentafluoropropionic acid, penta...	374 C18H31F5O2	959092-08-1 94



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100417\
Data File : BF099067.D
Acq On : 4 Oct 2017 15:24
Operator : SJ/JU
Sample : I5584-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

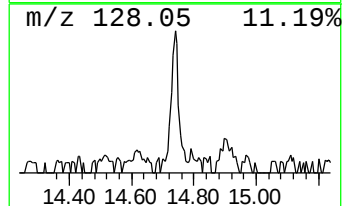
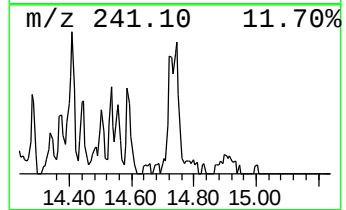
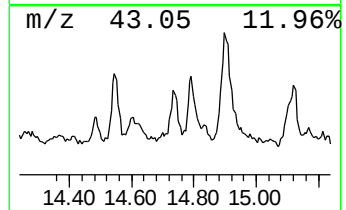
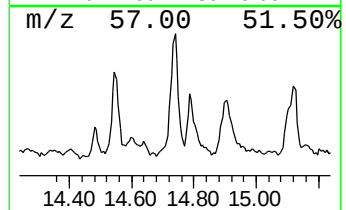
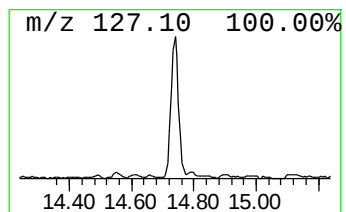
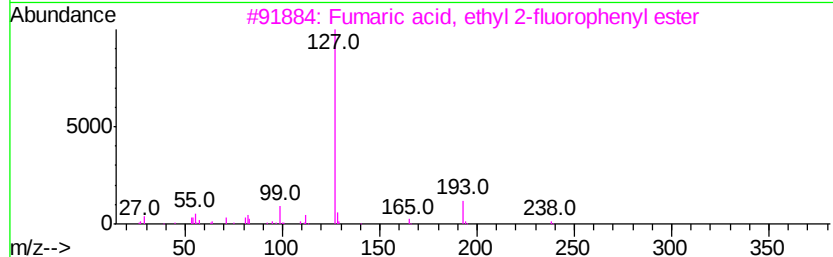
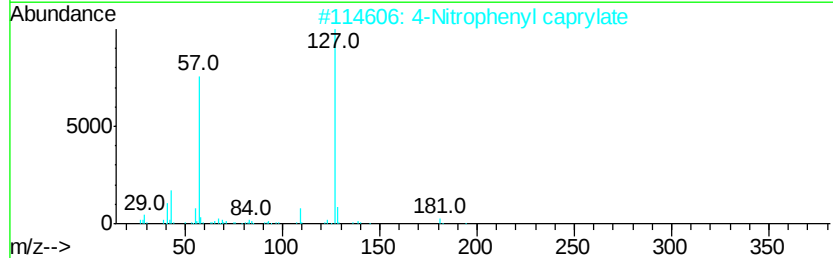
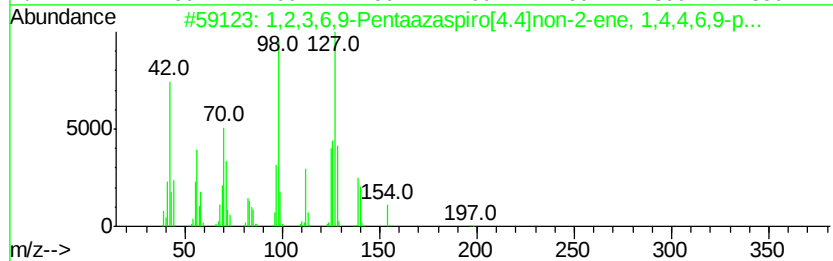
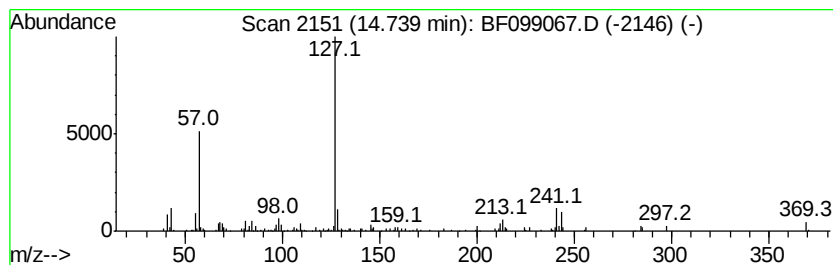
Instrument :
BNA_F
ClientSampleId :
TP-1-COMP

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 13 1,2,3,6,9-Pentaazaspiro[4.4... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.74	2.74 ng	251339	Chrysene-d12	14.03		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,3,6,9-Pentaazaspiro[4.4]non-...	197	C9H19N5	1000221-38-7	70	
2	4-Nitrophenyl caprylate	265	C14H19NO4	001956-10-1	53	
3	Fumaric acid, ethyl 2-fluorophen...	238	C12H11FO4	1000345-21-5	50	
4	Octanoic acid, 4-cyano-2,6-diiod...	497	C15H17I2NO2	003861-47-0	42	
5	Glutaric acid, 3,4-difluorobenzy...	356	C19H26F2O4	1000377-63-7	42	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100417\
Data File : BF099067.D
Acq On : 4 Oct 2017 15:24
Operator : SJ/JU
Sample : I5584-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

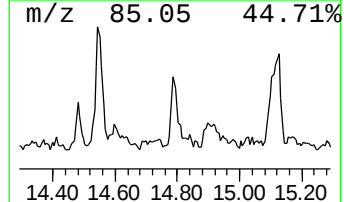
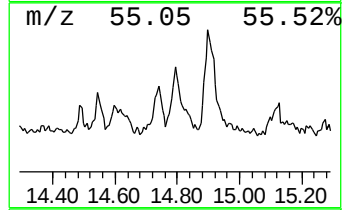
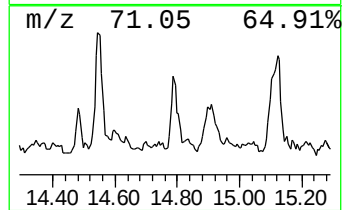
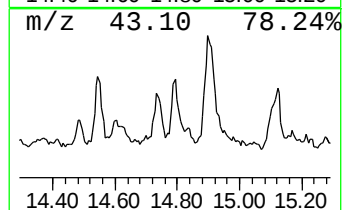
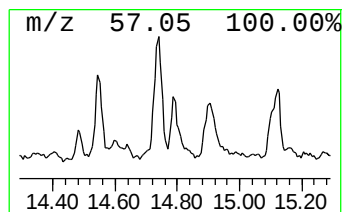
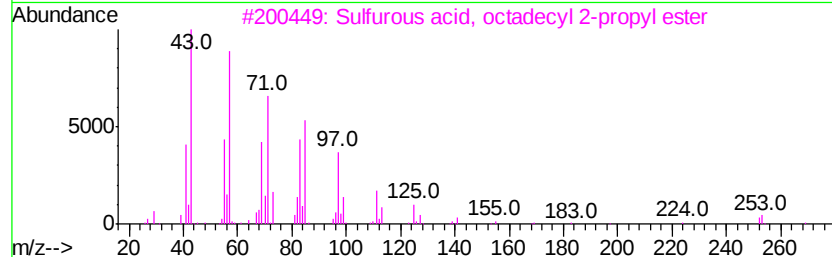
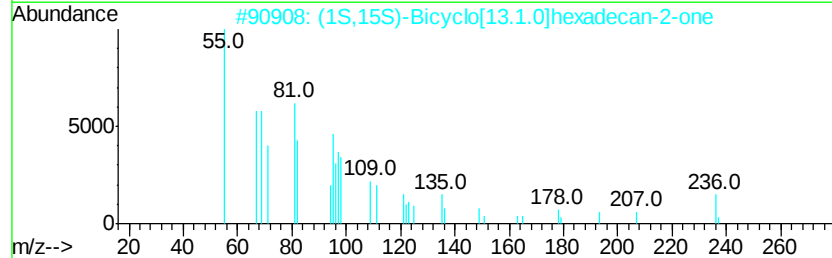
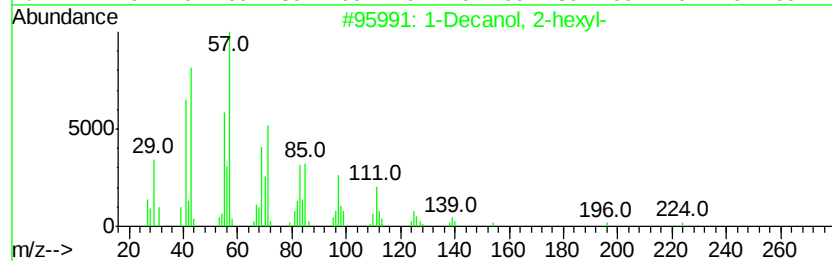
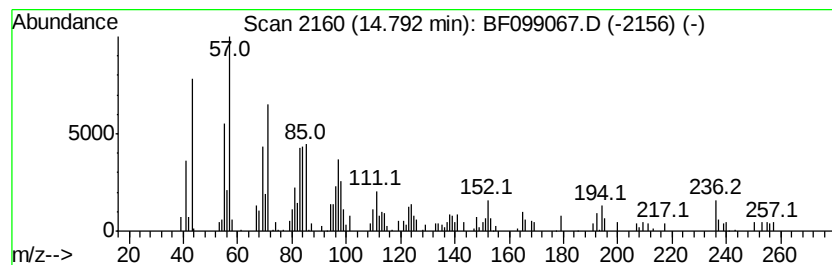
Instrument :
BNA_F
ClientSampleId :
TP-1-COMP

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 14 unknown14.79 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	4.44 ng	210985	Perylene-d12	15.50
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		1-Decanol, 2-hexyl-	242 C16H34O	002425-77-6 43
2		(1S,15S)-Bicyclo[13.1.0]hexadeca...	236 C16H28O	102572-89-4 38
3		Sulfurous acid, octadecyl 2-prop...	376 C21H44O3S	1000309-12-7 38
4		1-Dodecanol, 2-hexyl-	270 C18H38O	110225-00-8 38
5		Bromoacetic acid, octadecyl ester	390 C20H39BrO2	018992-03-5 30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100417\
Data File : BF099067.D
Acq On : 4 Oct 2017 15:24
Operator : SJ/JU
Sample : I5584-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

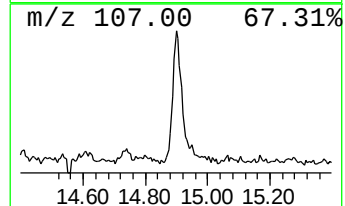
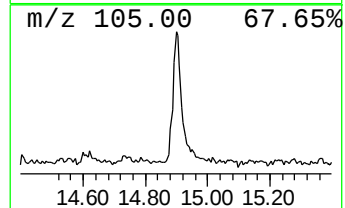
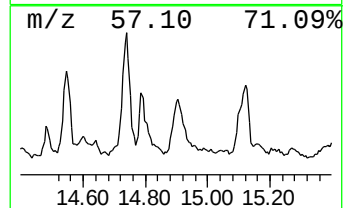
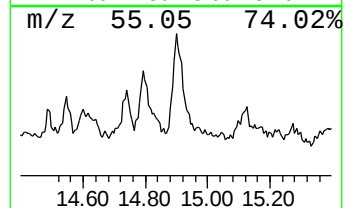
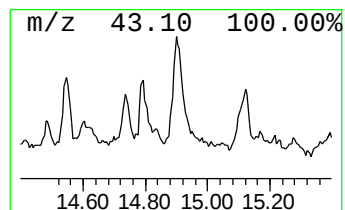
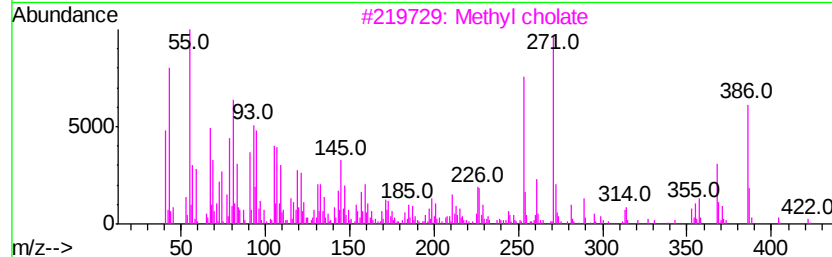
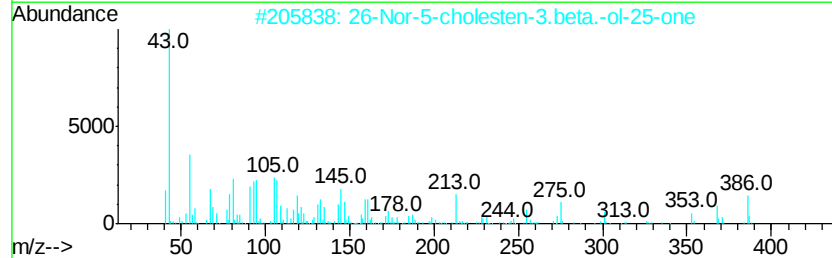
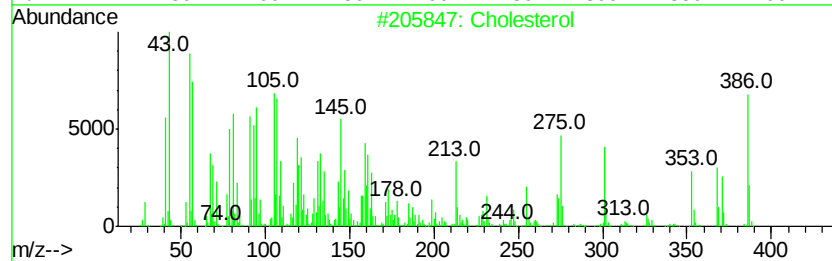
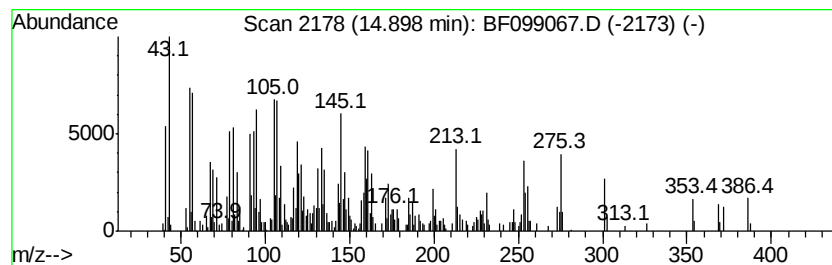
Instrument :
BNA_F
ClientSampleId :
TP-1-COMP

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 15 Cholesterol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.90	14.56 ng	691329	Perylene-d12	15.50	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholesterol	386	C27H46O	000057-88-5	99
2	26-Nor-5-cholesten-3.beta.-ol-25...	386	C26H42O2	007494-34-0	99
3	Methyl cholate	422	C25H42O5	001448-36-8	27
4	Cholesta-3,5-diene	368	C27H44	000747-90-0	14
5	3-n-Heptyl-7-methyl-9-(2,6,6-tri...	368	C26H40O	1000216-09-3	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100417\
Data File : BF099067.D
Acq On : 4 Oct 2017 15:24
Operator : SJ/JU
Sample : I5584-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1-COMP

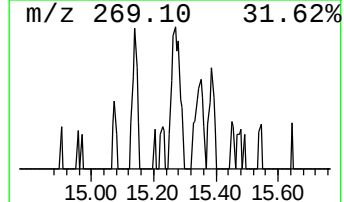
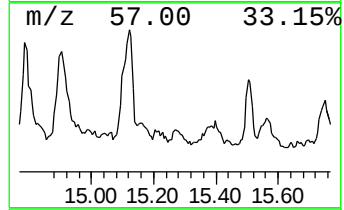
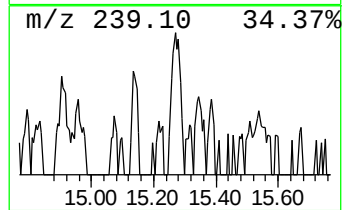
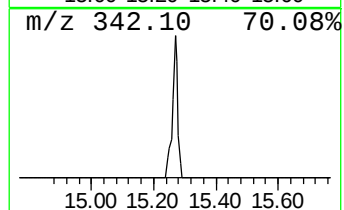
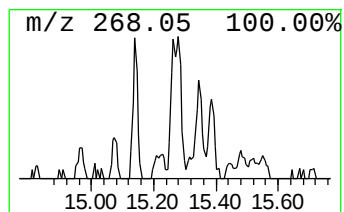
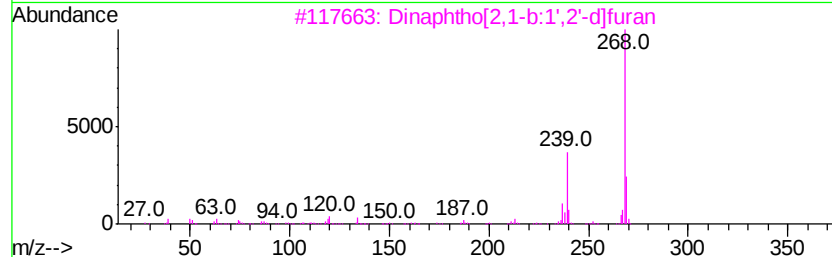
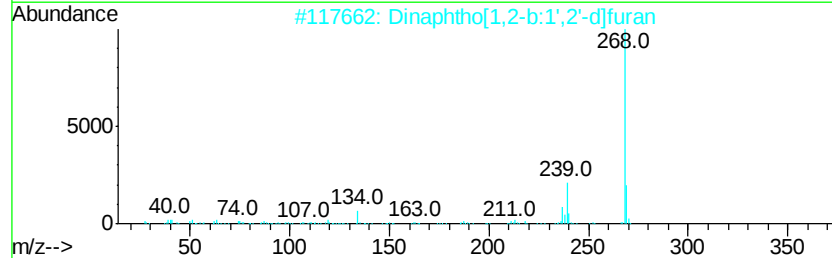
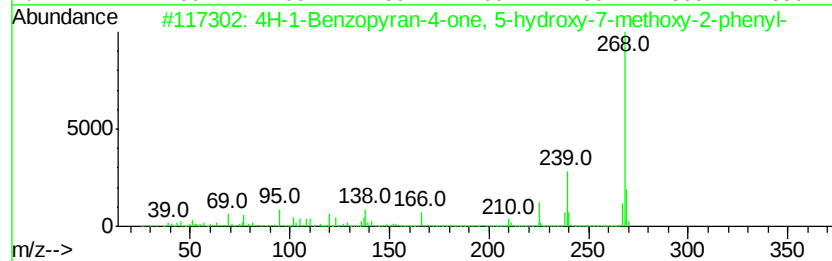
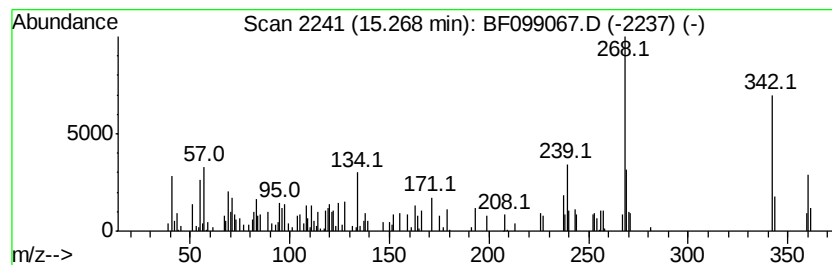
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown15.27 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.27	2.34 ng	111297	Perylene-d12	15.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4H-1-Benzopyran-4-one, 5-hydroxy...	268	C16H12O4	000520-28-5	45
2		Dinaphtho[1,2-b:1',2'-d]furan	268	C20H12O	000207-93-2	43
3		Dinaphtho[2,1-b:1',2'-d]furan	268	C20H12O	000194-63-8	43
4		Benzo(a)pyrene 4,5-oxide	268	C20H12O	037574-47-3	43
5		Tricyclo[3.3.1.1<3,7>]decane, tri...	268	C20H28	030541-56-1	38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100417\
Data File : BF099067.D
Acq On : 4 Oct 2017 15:24
Operator : SJ/JU
Sample : I5584-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1-COMP

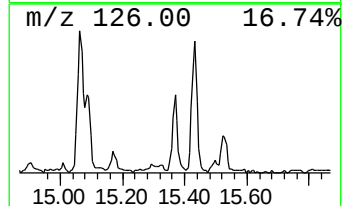
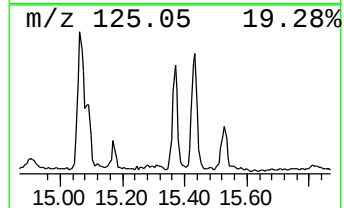
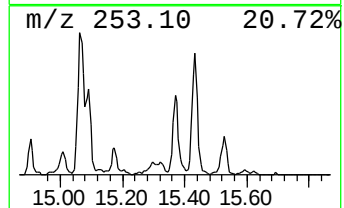
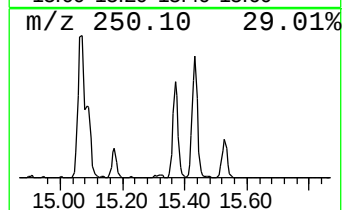
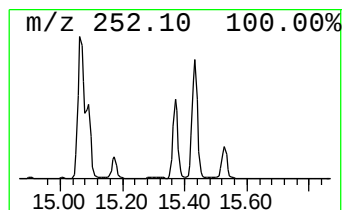
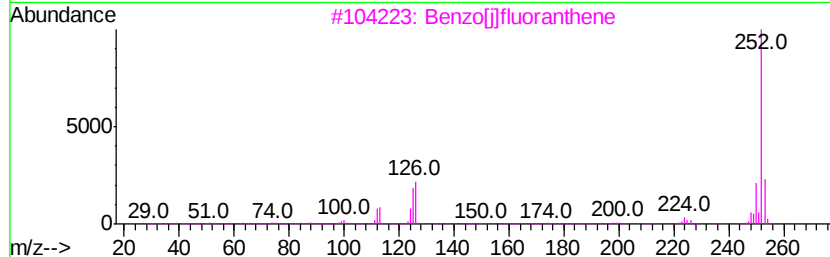
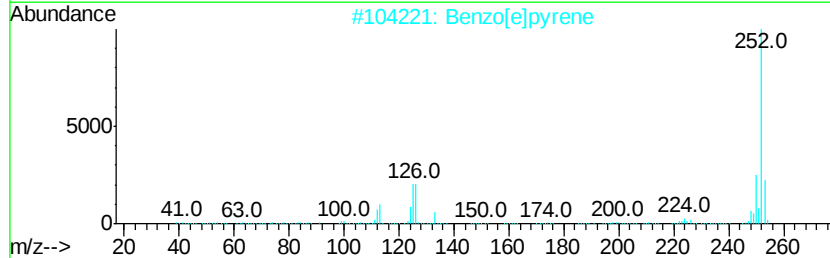
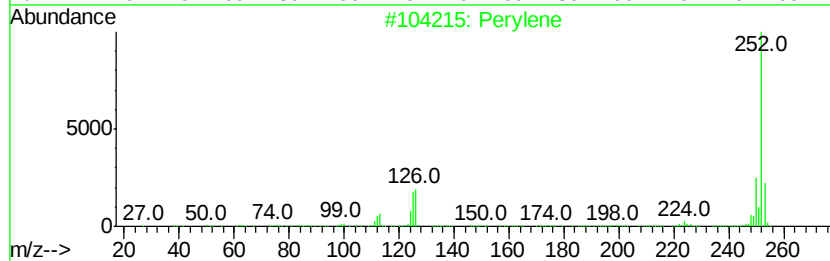
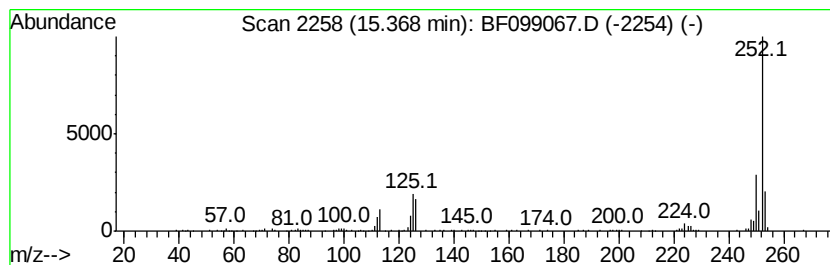
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Perylene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.37	5.53 ng	262468	Perylene-d12	15.50

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Perylene	252	C20H12	000198-55-0	99
2			Benzo[e]pyrene	252	C20H12	000192-97-2	98
3			Benzo[i]fluoranthene	252	C20H12	000205-82-3	98
4			Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	97
5			Benzo[a]pyrene	252	C20H12	000050-32-8	96



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100417\
Data File : BF099067.D
Acq On : 4 Oct 2017 15:24
Operator : SJ/JU
Sample : I5584-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1-COMP

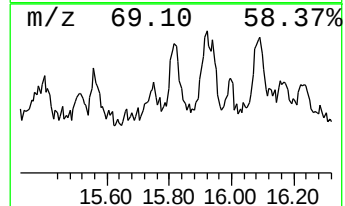
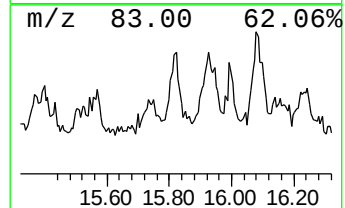
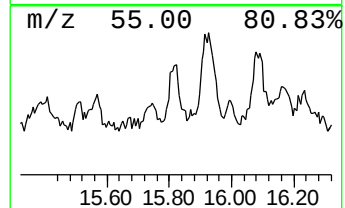
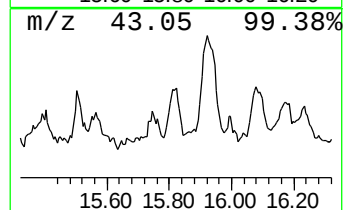
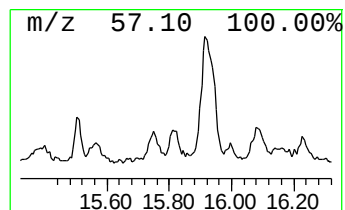
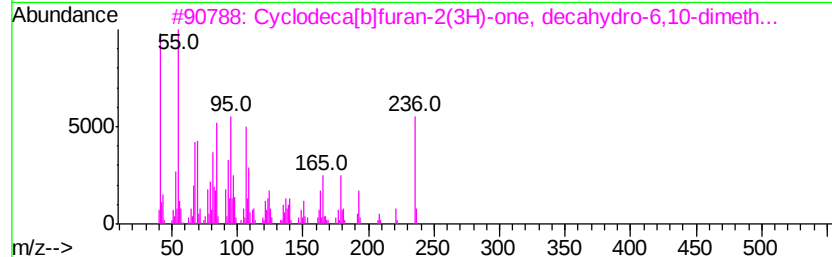
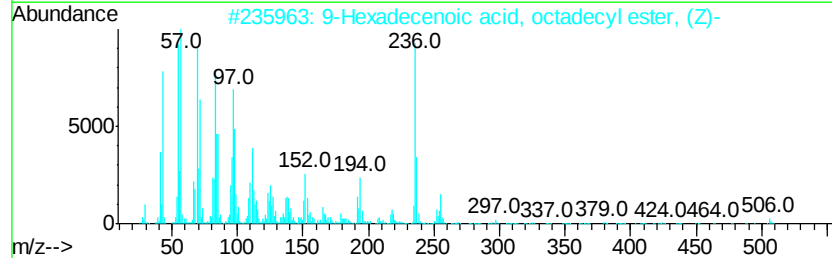
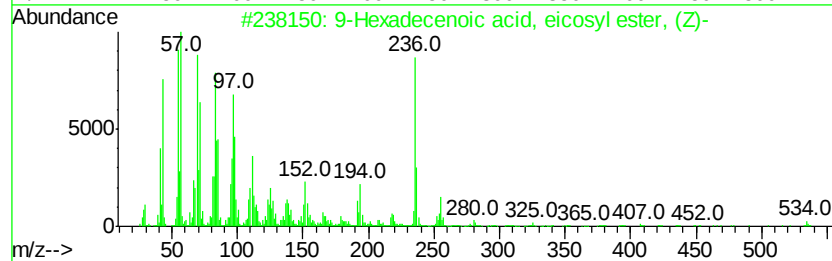
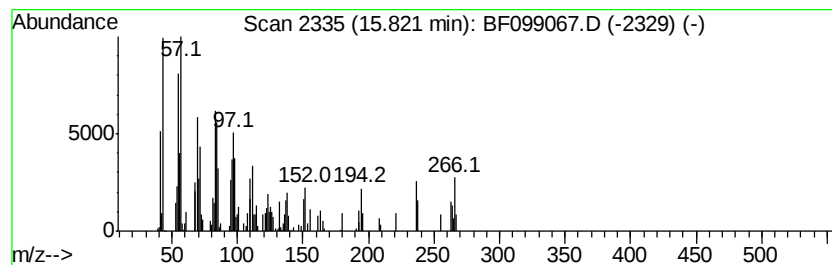
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 9-Hexadecenoic acid, eicosy... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.82	2.38 ng	113008	Perylene-d12	15.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Hexadecenoic acid, eicosyl est...	535	C36H70O2	022522-34-5	55
2		9-Hexadecenoic acid, octadecyl e...	507	C34H66O2	022393-84-6	55
3		Cyclodeca[b]furan-2(3H)-one, dec...	236	C15H24O2	054833-41-9	46
4		9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	45
5		cis-Vaccenic acid	282	C18H34O2	000506-17-2	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100417\
Data File : BF099067.D
Acq On : 4 Oct 2017 15:24
Operator : SJ/JU
Sample : I5584-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1-COMP

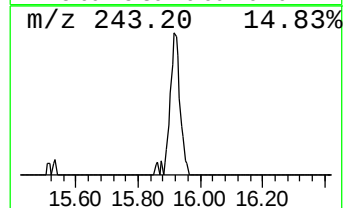
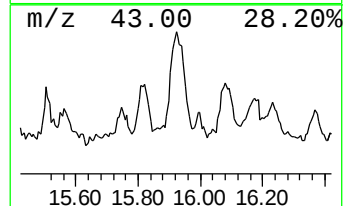
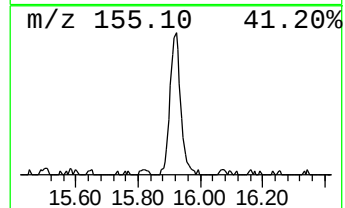
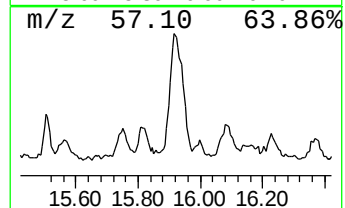
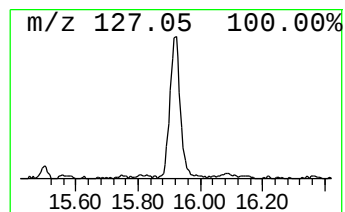
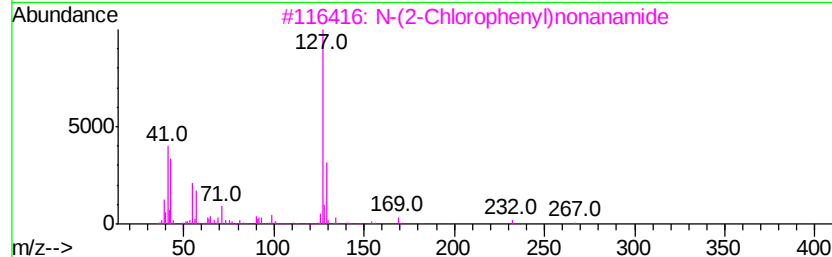
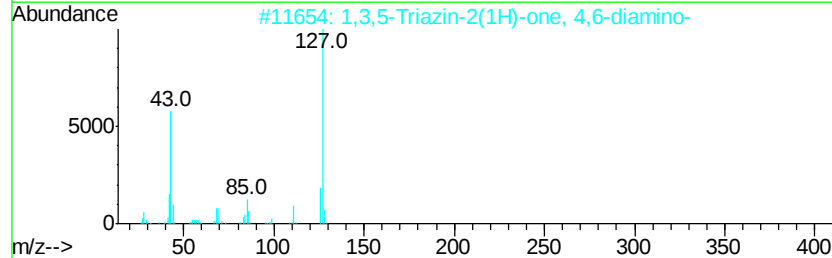
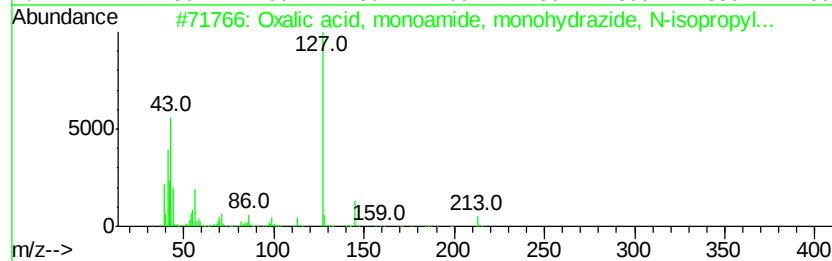
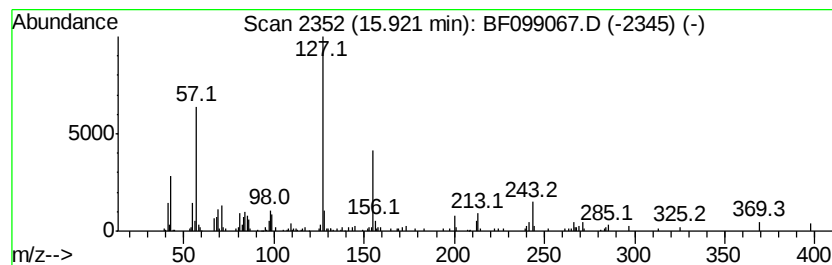
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 unknown15.92 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.92	8.22 ng	390416	Perylene-d12	15.50

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, monoamide, monohydr...	213	C10H19N3O2	1000265-20-0	43
2			1,3,5-Triazin-2(1H)-one, 4,6-dia...	127	C3H5N5O	000645-92-1	43
3			N-(2-Chlorophenyl)nonanamide	267	C15H22ClNO	143943-85-5	38
4			Fumaric acid, ethyl 2-isopropoxyv...	278	C15H18O5	1000344-83-7	38
5			Caprylic anhydride	270	C16H30O3	000623-66-5	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100417\
Data File : BF099067.D
Acq On : 4 Oct 2017 15:24
Operator : SJ/JU
Sample : I5584-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1-COMP

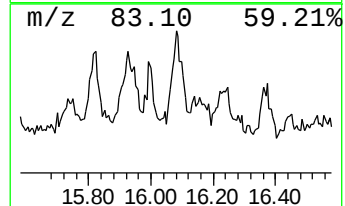
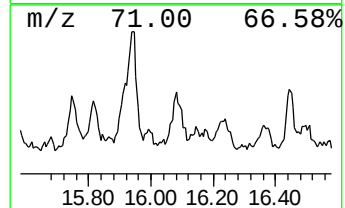
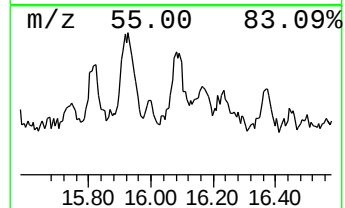
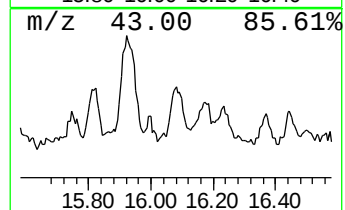
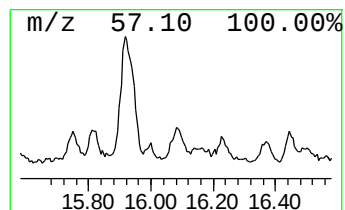
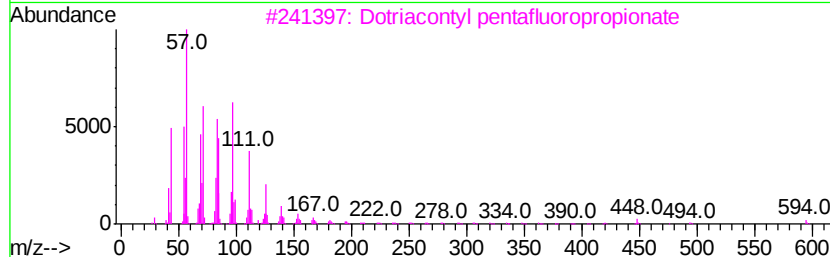
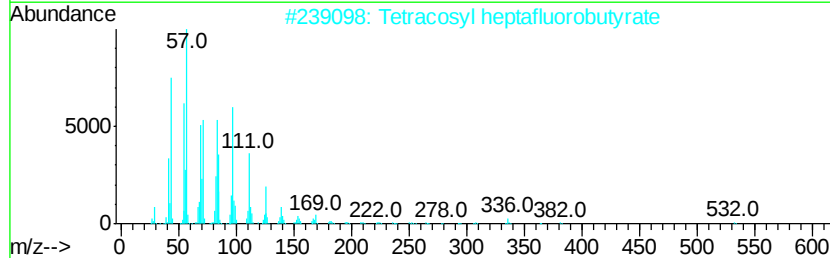
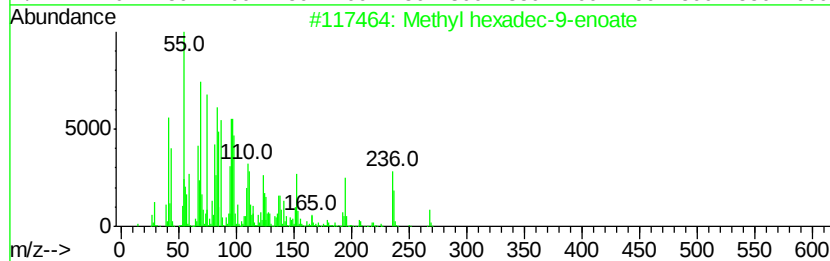
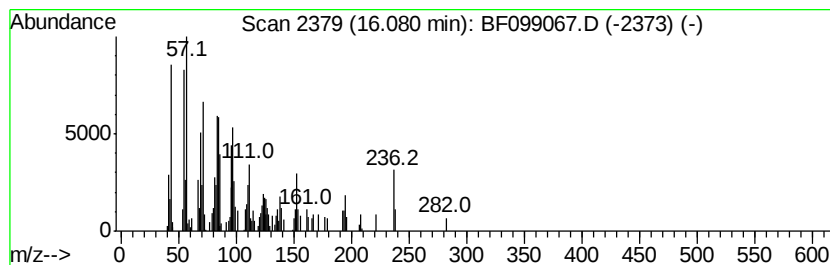
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 unknown16.08 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.08	3.33 ng	157997	Perylene-d12	15.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methyl hexadec-9-enoate	268	C17H32O2	010030-74-7	45
2		Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	42
3		Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1000351-81-4	42
4		Cyclopentane, (4-octyldodecyl)-	350	C25H50	005638-09-5	42
5		Octacosyl heptafluorobutyrate	606	C32H57F7O2	1000351-83-6	42



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100417\
 Data File : BF099067.D
 Acq On : 4 Oct 2017 15:24
 Operator : SJ/JU
 Sample : I5584-01
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-1-COMP

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...	2.16	9.3	ng	466711	1	6.86	1006170	20.0
2-Pentanone, 4-hy...	5.10	15.7	ng	787572	1	6.86	1006170	20.0
unknown6.64	6.64	79.3	ng	3990440	1	6.86	1006170	20.0
1-Decene	9.69	2.5	ng	177273	3	9.90	1448510	20.0
Tridecane	10.80	2.3	ng	170312	4	11.39	1475530	20.0
Cyclododecane	11.60	2.5	ng	182373	4	11.39	1475530	20.0
n-Hexadecanoic acid	11.91	3.9	ng	290175	4	11.39	1475530	20.0
4H-Cyclopenta[def...	12.00	4.0	ng	291110	4	11.39	1475530	20.0
13-Docosenamide, ...	12.14	81.3	ng	6001500	4	11.39	1475530	20.0
Squalene	12.47	23.8	ng	1755530	4	11.39	1475530	20.0
Behenic alcohol	13.85	5.7	ng	521804	5	14.03	1832380	20.0
1,2,3,6,9-Pentaaz...	14.74	2.7	ng	251339	5	14.03	1832380	20.0
unknown14.79	14.79	4.4	ng	210985	6	15.50	949536	20.0
Cholesterol	14.90	14.6	ng	691329	6	15.50	949536	20.0
unknown15.27	15.27	2.3	ng	111297	6	15.50	949536	20.0
Perylene	15.37	5.5	ng	262468	6	15.50	949536	20.0
9-Hexadecenoic ac...	15.82	2.4	ng	113008	6	15.50	949536	20.0
unknown15.92	15.92	8.2	ng	390416	6	15.50	949536	20.0
unknown16.08	16.08	3.3	ng	157997	6	15.50	949536	20.0