

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100918\
 Data File : BF109716.D
 Acq On : 10 Oct 2018 1:07
 Operator : JU/SJ
 Sample : J5326-39
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FL-PH-3-STONE

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.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	4.893	474	477	486	rBV	36946	51294	2.96%	0.351%
2	5.316	545	549	569	rBV	946213	1243623	71.85%	8.515%
3	6.345	720	724	741	rBV	1000220	1437665	83.06%	9.843%
4	6.469	741	745	771	rVB	1300885	1584097	91.52%	10.846%
5	6.698	781	784	795	rBV	289033	401427	23.19%	2.748%
6	6.851	806	810	847	rVB	1186413	1225323	70.79%	8.390%
7	7.257	876	879	913	rBV	595532	953939	55.11%	6.531%
8	7.975	998	1001	1019	rBV	397425	514780	29.74%	3.525%
9	9.051	1180	1184	1212	rBV	1510993	1730819	100.00%	11.851%
10	9.445	1247	1251	1260	rBV	87257	91077	5.26%	0.624%
11	9.722	1294	1298	1307	rBV	509613	506707	29.28%	3.469%
12	10.510	1428	1432	1450	rBV	556647	781875	45.17%	5.353%
13	11.198	1546	1549	1566	rBV	346265	475421	27.47%	3.255%
14	11.739	1638	1641	1650	rBV3	20204	32740	1.89%	0.224%
15	12.410	1751	1755	1764	rBV	46797	60689	3.51%	0.416%
16	12.633	1788	1793	1797	rBV	43133	54102	3.13%	0.370%
17	12.780	1814	1818	1830	rBV	1383569	1398881	80.82%	9.578%
18	13.686	1968	1972	1987	rBV2	74512	169970	9.82%	1.164%
19	13.827	1990	1996	2009	rVB	510491	615172	35.54%	4.212%
20	13.998	2022	2025	2028	rBV	21119	19995	1.16%	0.137%
21	14.304	2073	2077	2079	rBV	41391	42492	2.46%	0.291%
22	14.339	2079	2083	2088	rVB7	11138	21470	1.24%	0.147%
23	14.592	2123	2126	2129	rVB	47380	43874	2.53%	0.300%
24	14.662	2135	2138	2142	rBV	56310	55341	3.20%	0.379%
25	14.727	2146	2149	2152	rVB2	18444	17682	1.02%	0.121%
26	14.839	2163	2168	2175	rBV	27822	61814	3.57%	0.423%
27	14.904	2175	2179	2183	rVV	96630	100254	5.79%	0.686%
28	15.115	2210	2215	2218	rBV	14744	20180	1.17%	0.138%
29	15.174	2221	2225	2229	rVB2	15709	22278	1.29%	0.153%
30	15.227	2229	2234	2247	rBV	274085	488747	28.24%	3.346%
31	15.433	2266	2269	2277	rVB5	21458	33787	1.95%	0.231%
32	15.645	2300	2305	2311	rBV	83333	117288	6.78%	0.803%
33	15.745	2313	2322	2329	rBV9	13712	48158	2.78%	0.330%
34	16.098	2377	2382	2387	rBV2	38115	60590	3.50%	0.415%

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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 >
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35	16.362	2422	2427	2433	rVB6	17259	28634	1.65%	0.196%
36	16.633	2469	2473	2481	rVB2	25431	51886	3.00%	0.355%
37	16.862	2507	2512	2517	rVB5	22953	41311	2.39%	0.283%

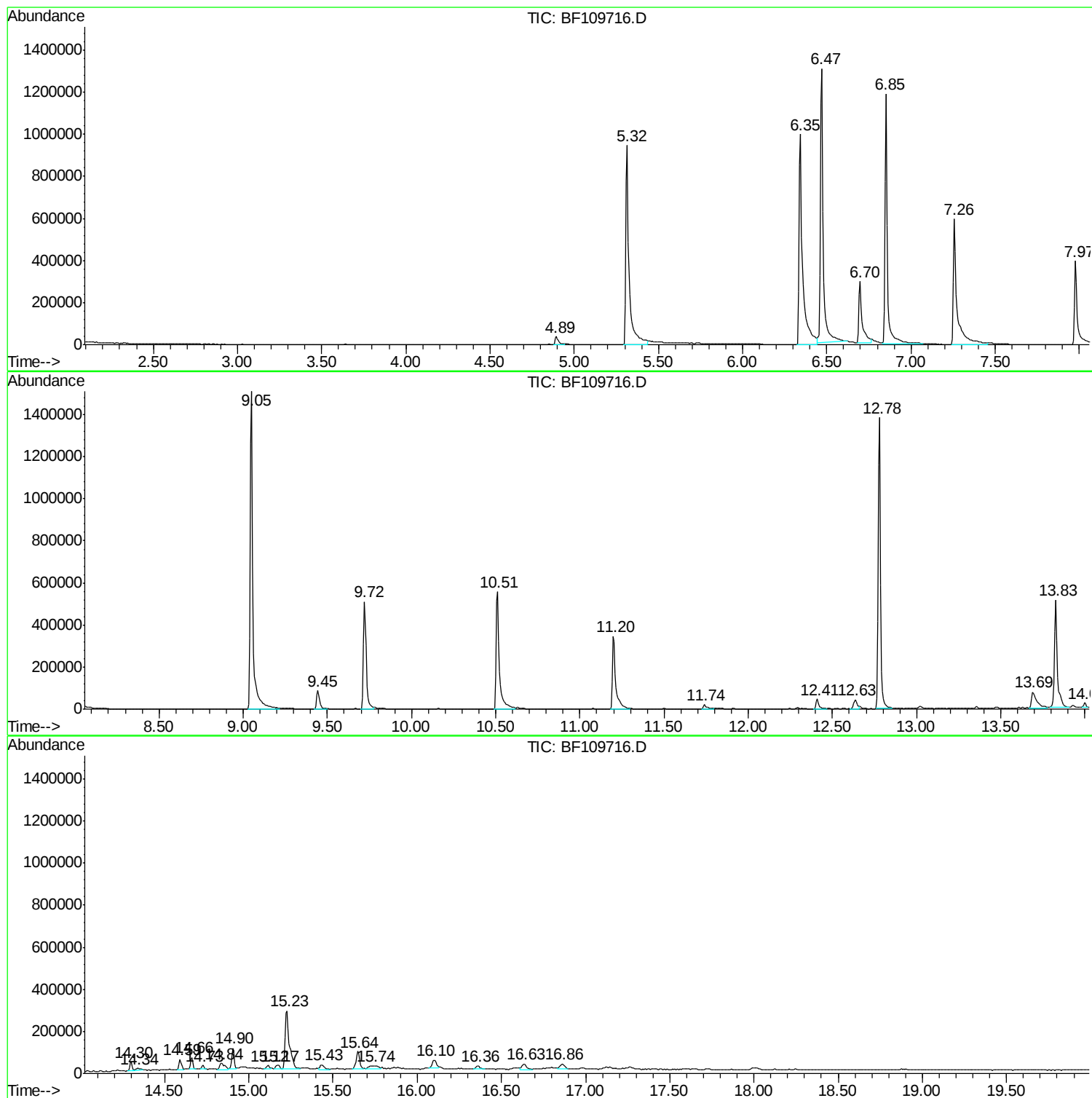
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF100818.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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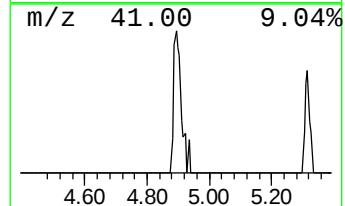
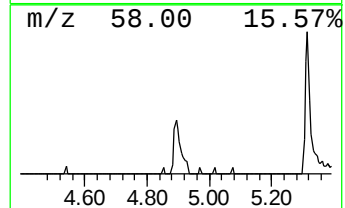
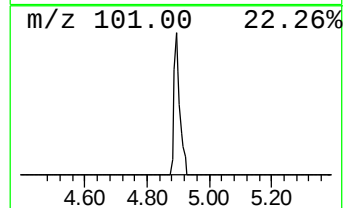
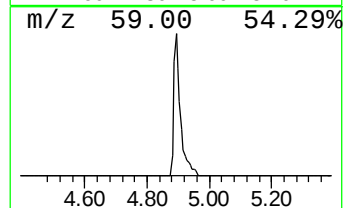
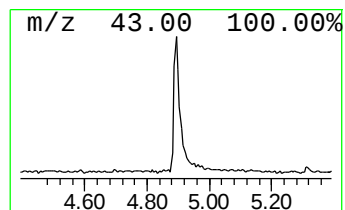
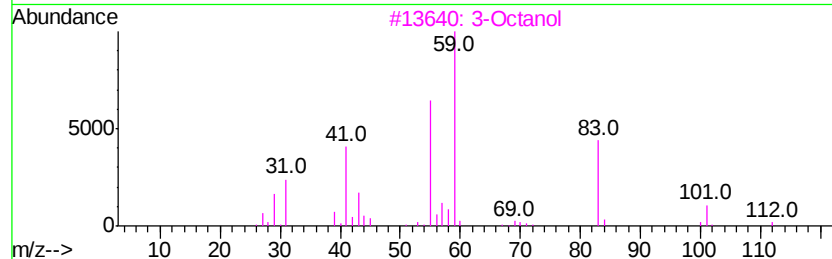
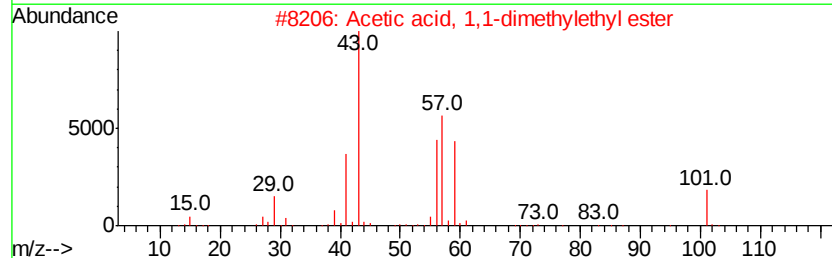
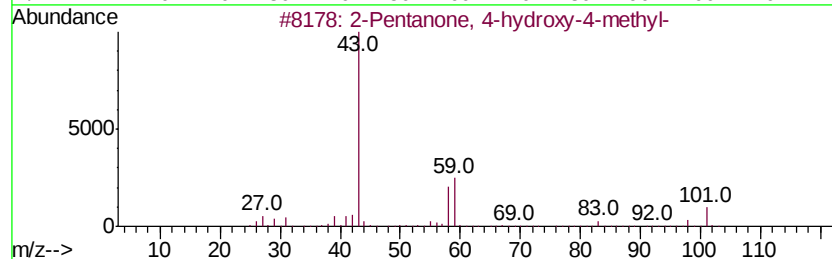
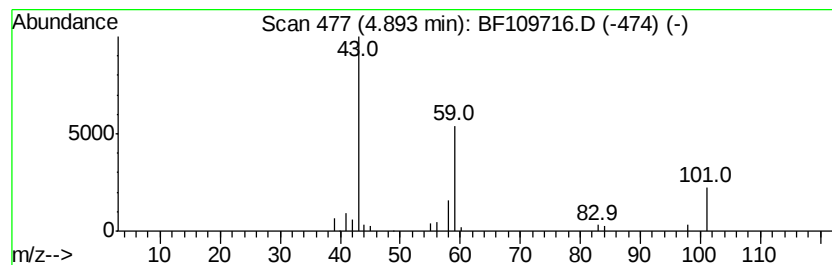
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	2.56 ng	51294	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			3-Octanol	130	C8H18O	000589-98-0	25
4			3-Hexanol	102	C6H14O	000623-37-0	25
5			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23



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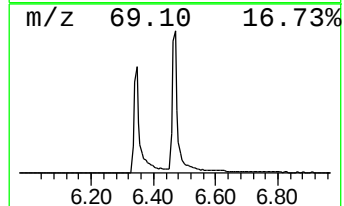
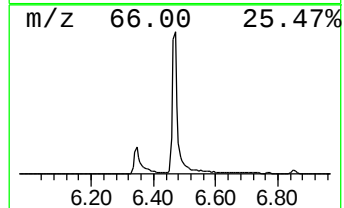
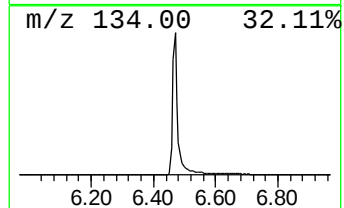
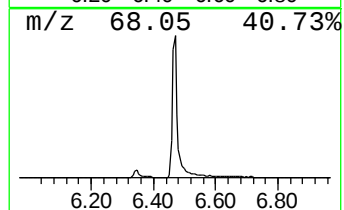
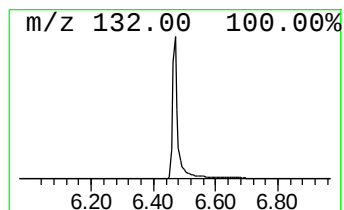
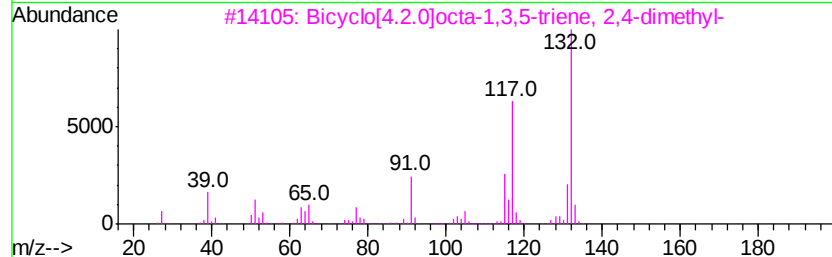
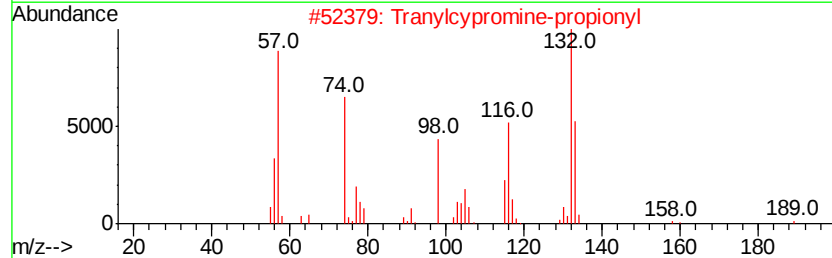
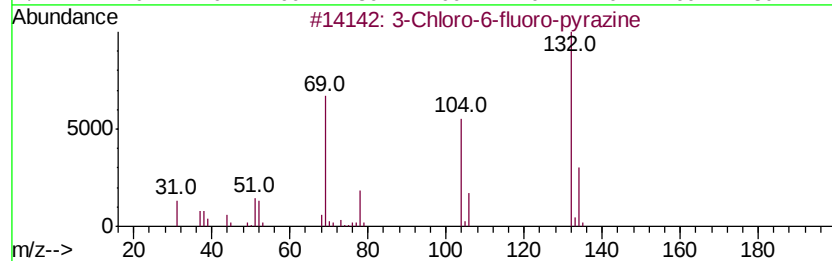
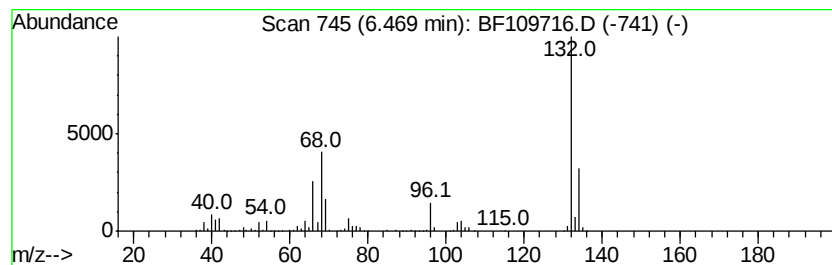
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Peak Number 2 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	78.92 ng	1584100	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
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		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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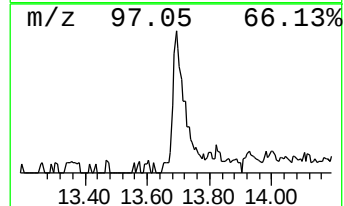
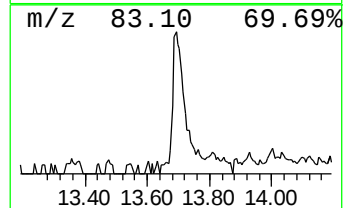
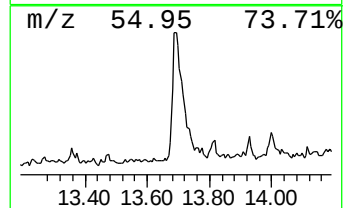
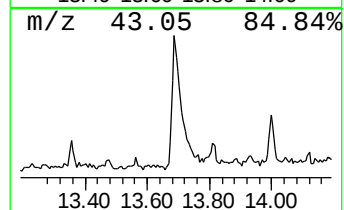
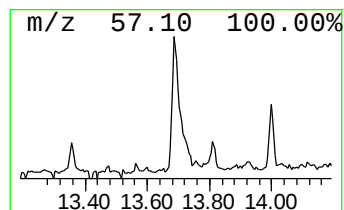
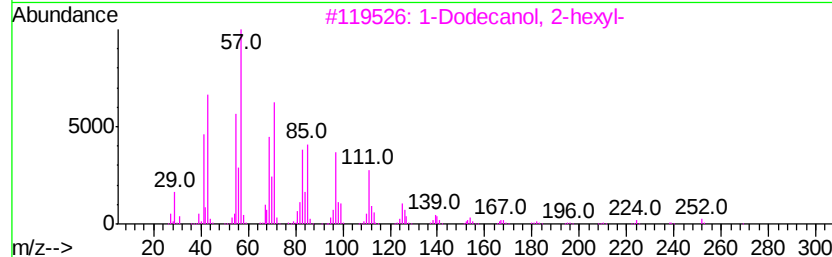
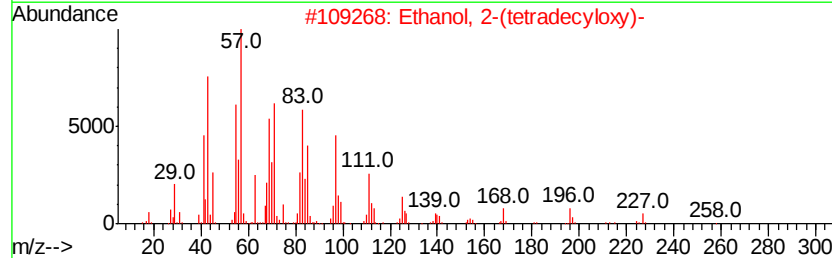
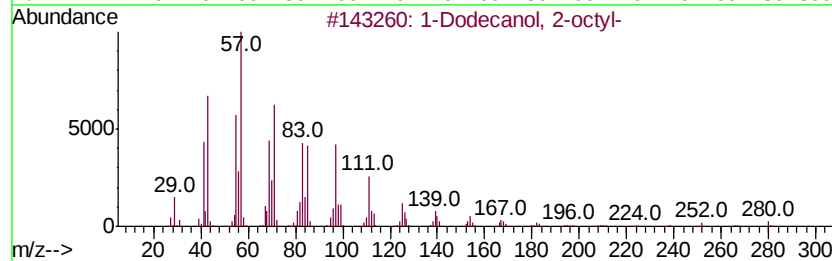
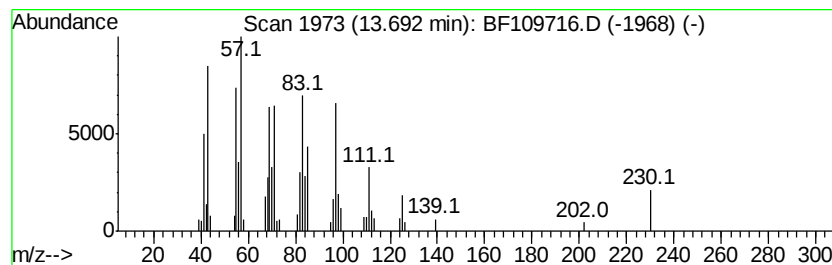
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 1-Dodecanol, 2-octyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.69	5.53 ng	169970	Chrysene-d12	13.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	90
2		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
3		1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	87
4		Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	87
5		Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	87



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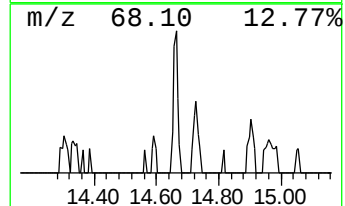
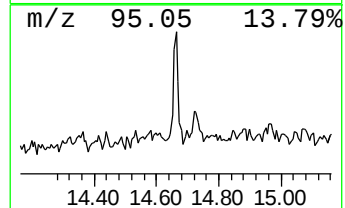
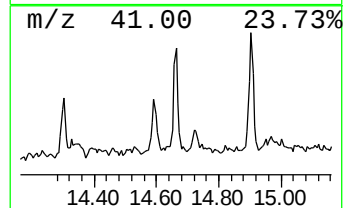
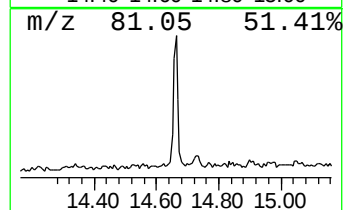
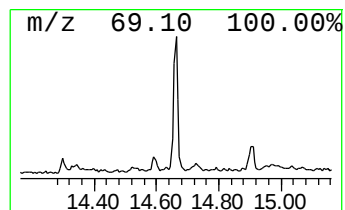
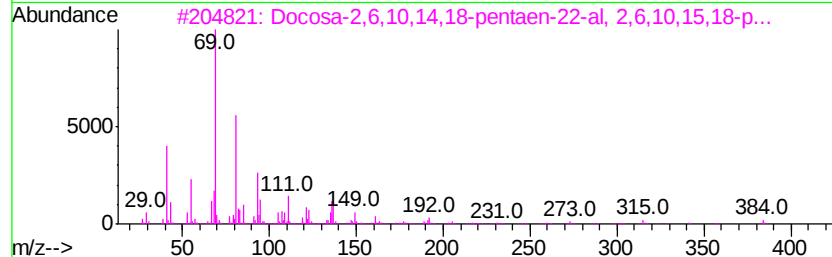
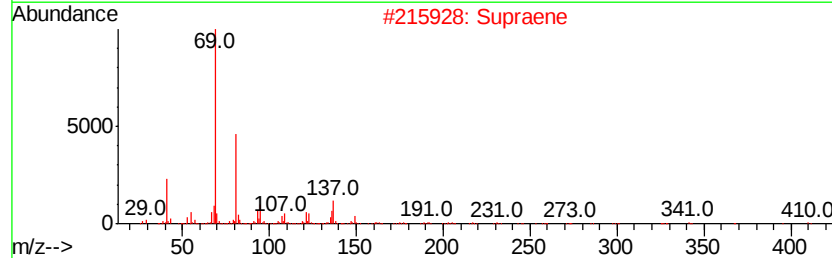
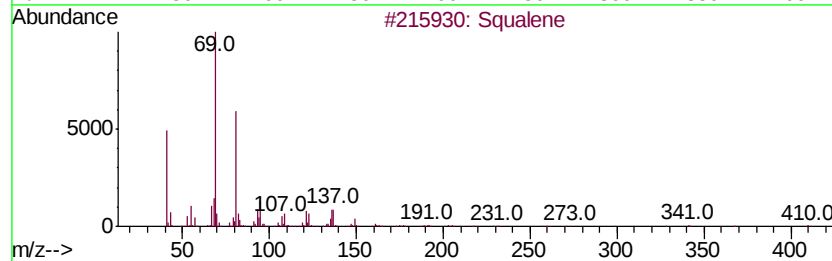
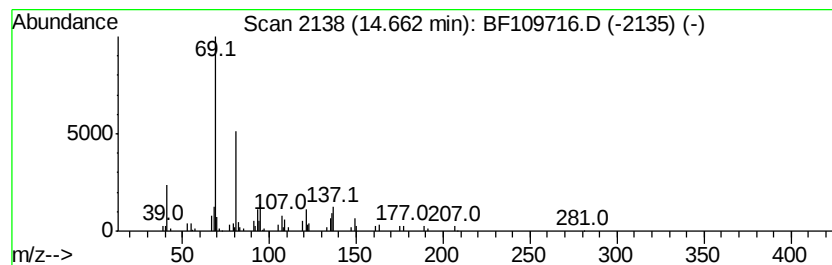
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Peak Number 5 Squalene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	2.26 ng	55341	Perylene-d12	15.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	90
2		Supraene	410	C30H50	007683-64-9	87
3		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	86
4		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	64
5		trans-Farnesol	222	C15H26O	000106-28-5	59



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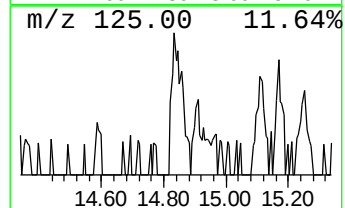
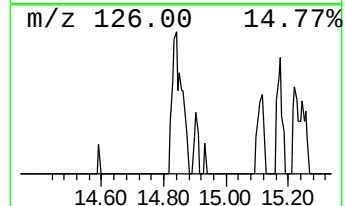
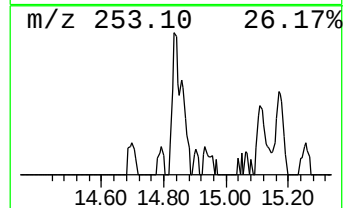
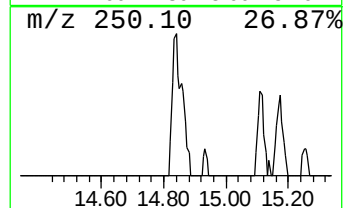
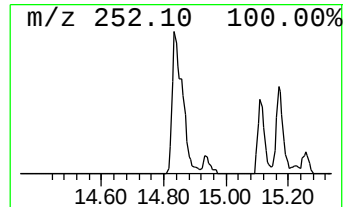
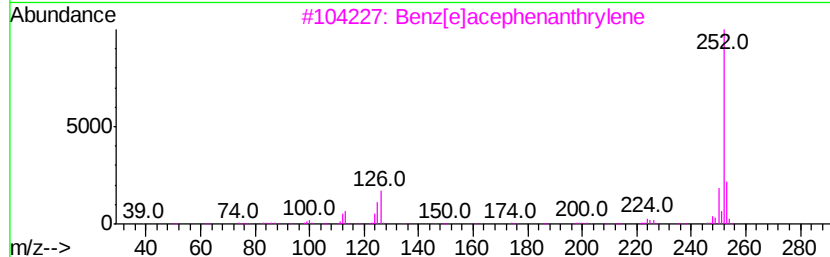
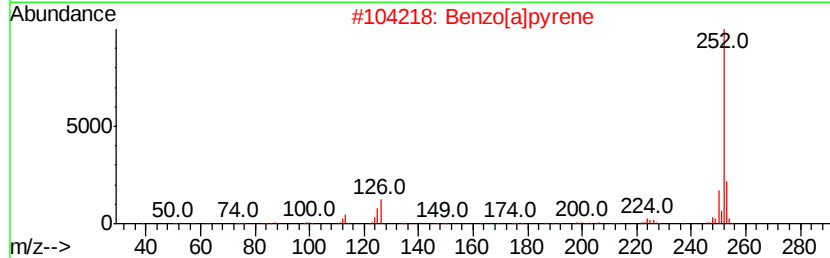
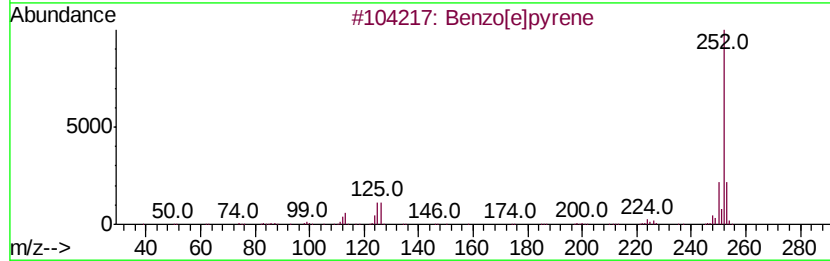
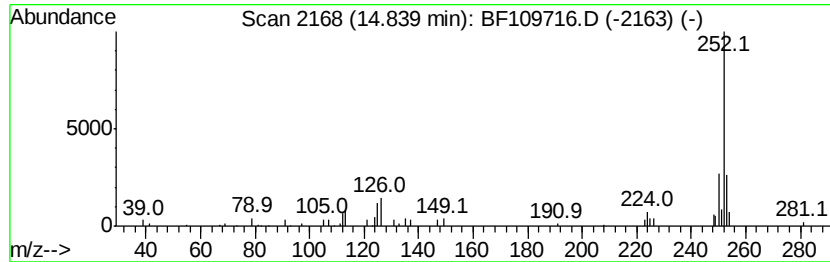
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.84	2.53 ng	61814	Perylene-d12	15.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	93
2	Benzo[a]pyrene	252	C20H12	000050-32-8	87
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	87
4	Perylene	252	C20H12	000198-55-0	83
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	81



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100918\
Data File : BF109716.D
Acq On : 10 Oct 2018 1:07
Operator : JU/SJ
Sample : J5326-39
Misc :
ALS Vial : 20 Sample Multiplier: 1

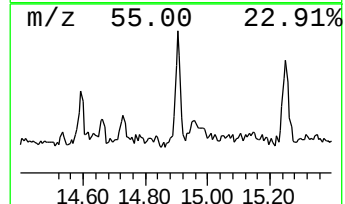
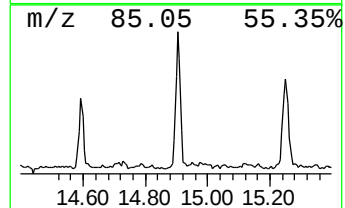
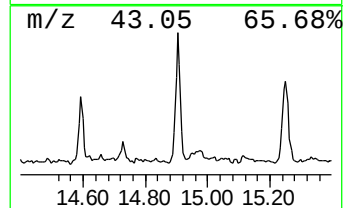
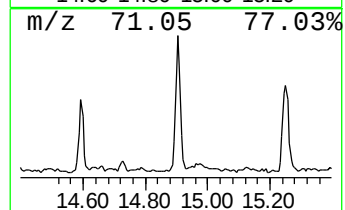
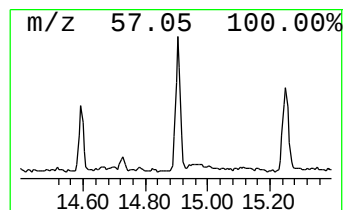
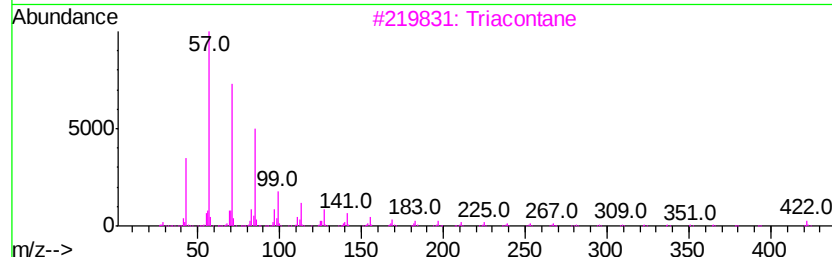
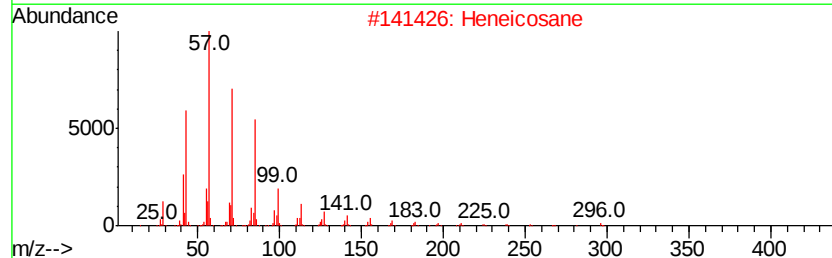
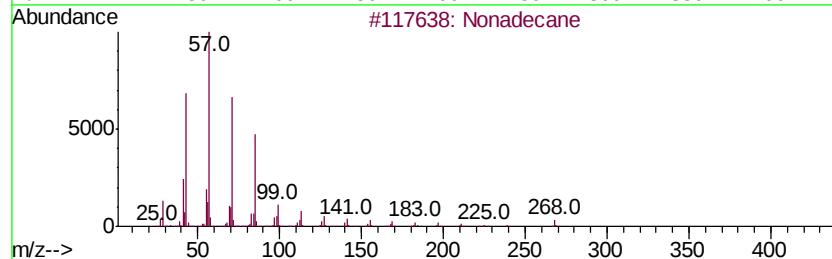
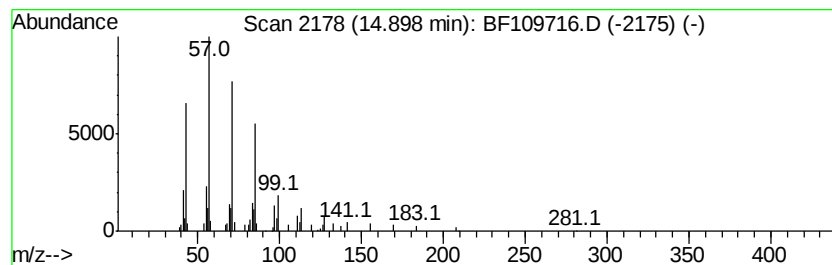
Instrument :
BNA_F
ClientSampleId :
FL-PH-3-STONE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Nonadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.90	4.10 ng	100254	Perylene-d12		15.23
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	96
2	Heneicosane	296	C21H44	000629-94-7	91
3	Triacontane	422	C30H62	000638-68-6	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100918\
Data File : BF109716.D
Acq On : 10 Oct 2018 1:07
Operator : JU/SJ
Sample : J5326-39
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FL-PH-3-STONE

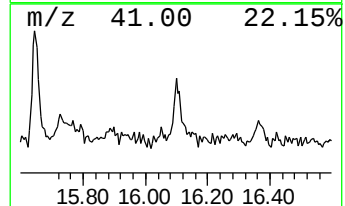
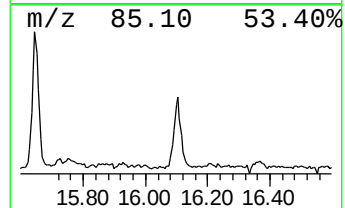
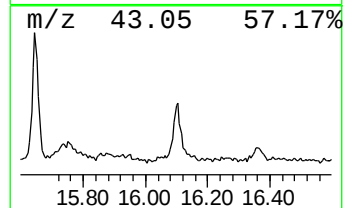
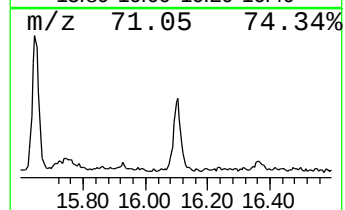
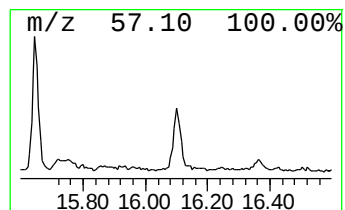
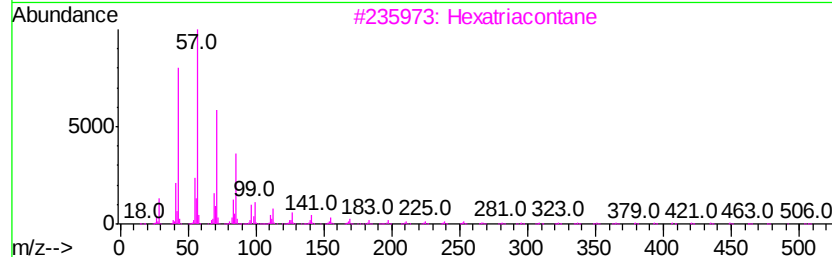
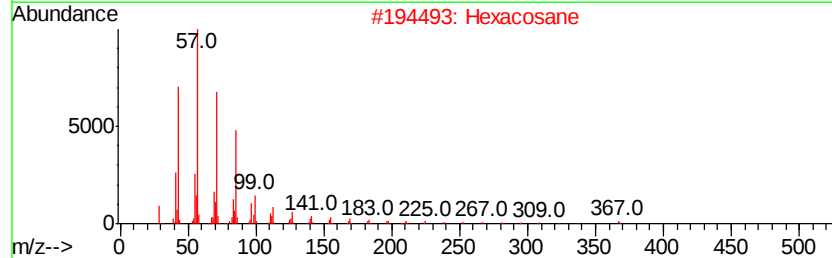
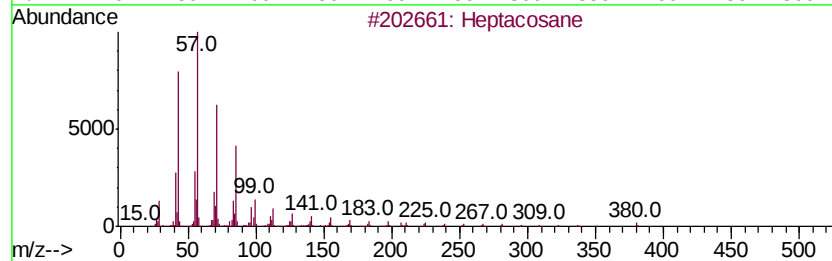
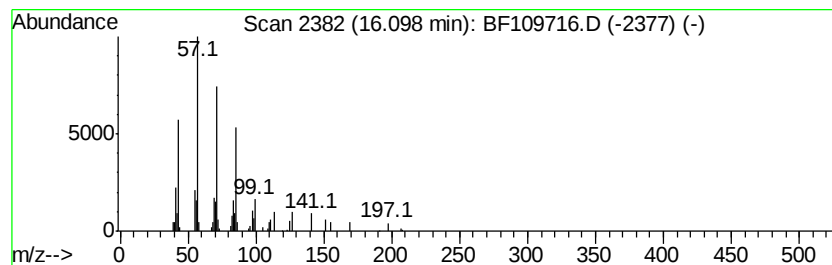
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.10	2.48 ng	60590	Perylene-d12	15.23

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	91
2	Hexacosane		366	C26H54	000630-01-3	91
3	Hexatriacontane		507	C36H74	000630-06-8	91
4	2-methyloctacosane		408	C29H60	1000376-72-8	91
5	Heneicosane		296	C21H44	000629-94-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100918\
Data File : BF109716.D
Acq On : 10 Oct 2018 1:07
Operator : JU/SJ
Sample : J5326-39
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FL-PH-3-STONE

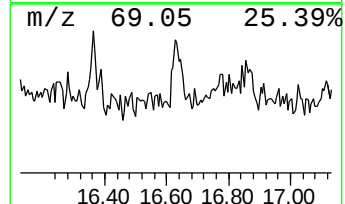
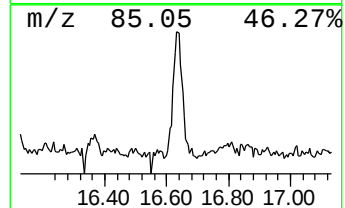
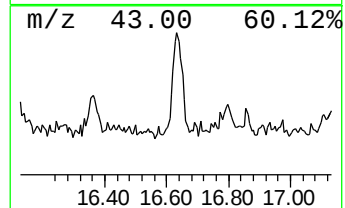
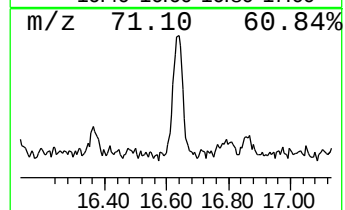
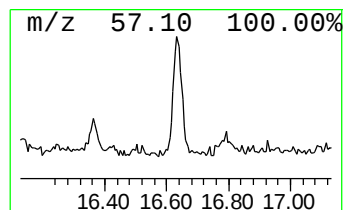
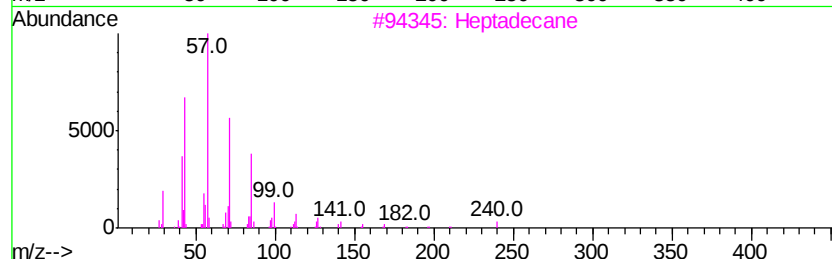
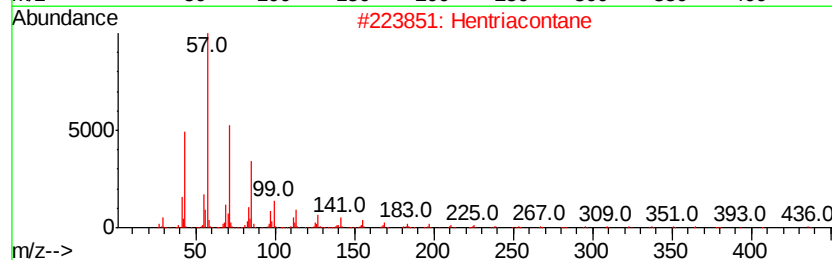
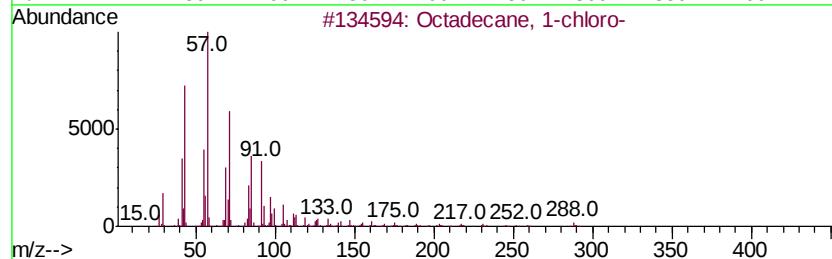
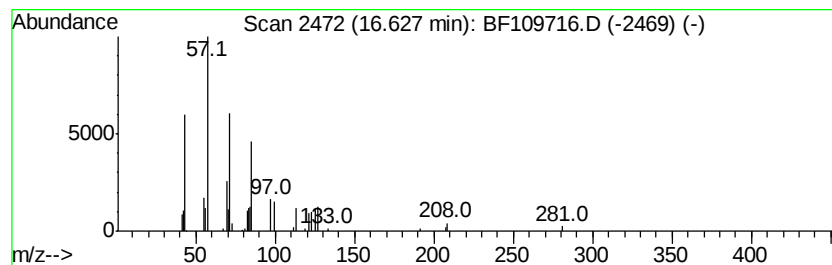
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octadecane, 1-chloro- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.63	2.12 ng	51886	Perylene-d12	15.23

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	83
2			Hentriacontane	437	C31H64	000630-04-6	72
3			Heptadecane	240	C17H36	000629-78-7	59
4			Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	59
5			Undecane	156	C11H24	001120-21-4	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF100918\
Data File : BF109716.D
Acq On : 10 Oct 2018 1:07
Operator : JU/SJ
Sample : J5326-39
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FL-PH-3-STONE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.89	2.6	ng	51294	1	6.70	401427	20.0
unknown6.47	6.47	78.9	ng	1584100	1	6.70	401427	20.0
1-Dodecanol, 2-oc...	13.69	5.5	ng	169970	5	13.83	615172	20.0
Squalene	14.66	2.3	ng	55341	6	15.23	488747	20.0
Benzo[e]pyrene	14.84	2.5	ng	61814	6	15.23	488747	20.0
Nonadecane	14.90	4.1	ng	100254	6	15.23	488747	20.0
Heptacosane	16.10	2.5	ng	60590	6	15.23	488747	20.0
Octadecane, 1-chl...	16.63	2.1	ng	51886	6	15.23	488747	20.0