

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF062818\
 Data File : BF106918.D
 Acq On : 28 Jun 2018 14:10
 Operator : JU/SJ
 Sample : J3570-05
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20180375-COMPOSITE-CS-1A-ELU

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-BF061918.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	5.184	481	484	492	rBV	57021	59335	2.61%	0.355%
2	5.590	549	553	563	rBV	1058161	912197	40.16%	5.460%
3	6.589	719	723	733	rVB	809334	751338	33.08%	4.497%
4	6.731	742	747	750	rBV	1603155	1520382	66.94%	9.101%
5	6.954	781	785	788	rBV	436400	390800	17.21%	2.339%
6	7.107	807	811	815	rBV	1479096	1421375	62.58%	8.508%
7	7.354	848	853	859	rVB	33509	28528	1.26%	0.171%
8	7.519	873	881	884	rBV	1187013	1183962	52.13%	7.087%
9	7.672	904	907	913	rVB2	27665	27672	1.22%	0.166%
10	8.236	998	1003	1008	rBV	566202	501557	22.08%	3.002%
11	9.313	1179	1186	1189	rBV	2257160	2201030	96.91%	13.175%
12	9.454	1207	1210	1215	rBV3	26665	25754	1.13%	0.154%
13	9.701	1247	1252	1257	rBV	285806	244206	10.75%	1.462%
14	9.901	1282	1286	1288	rBV	48796	38830	1.71%	0.232%
15	9.995	1298	1302	1308	rVB	703460	605747	26.67%	3.626%
16	10.401	1368	1371	1374	rVB	103877	85841	3.78%	0.514%
17	10.536	1391	1394	1397	rVB2	34149	31703	1.40%	0.190%
18	10.624	1404	1409	1411	rBV	34890	42864	1.89%	0.257%
19	10.654	1411	1414	1417	rBV	269561	201260	8.86%	1.205%
20	10.789	1433	1437	1441	rBV	1539858	1516792	66.78%	9.079%
21	10.842	1444	1446	1449	rVV	77708	72204	3.18%	0.432%
22	10.877	1449	1452	1462	rVB2	90591	143963	6.34%	0.862%
23	10.960	1462	1466	1468	rBV	30733	34949	1.54%	0.209%
24	10.989	1468	1471	1474	rVB2	32246	36560	1.61%	0.219%
25	11.024	1474	1477	1479	rBV2	38827	36004	1.59%	0.216%
26	11.172	1499	1502	1505	rBV	31964	31327	1.38%	0.188%
27	11.324	1526	1528	1530	rBV	43082	29471	1.30%	0.176%
28	11.354	1530	1533	1540	rVB2	47392	57940	2.55%	0.347%
29	11.489	1552	1556	1559	rBV	768797	671375	29.56%	4.019%
30	11.636	1578	1581	1584	rBV	77383	69954	3.08%	0.419%
31	12.036	1647	1649	1654	rBV2	53134	51521	2.27%	0.308%
32	12.495	1725	1727	1732	rBV2	42780	53747	2.37%	0.322%
33	12.654	1752	1754	1758	rBV4	17621	28772	1.27%	0.172%
34	12.948	1802	1804	1810	rBV2	45160	53286	2.35%	0.319%

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

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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.077	1821	1826	1829	rBV	2237410	2271208	100.00%	13.595%
36	13.277	1858	1860	1863	rVB2	33872	30431	1.34%	0.182%
37	13.618	1916	1918	1922	rVB2	42991	39567	1.74%	0.237%
38	13.954	1972	1975	1983	rBV	94532	134537	5.92%	0.805%
39	14.018	1984	1986	1988	rBV2	30875	31109	1.37%	0.186%
40	14.148	2004	2008	2011	rVB	557954	535760	23.59%	3.207%
41	15.001	2150	2153	2156	rVB	61737	58496	2.58%	0.350%
42	15.695	2266	2271	2276	rVB	344392	442966	19.50%	2.651%

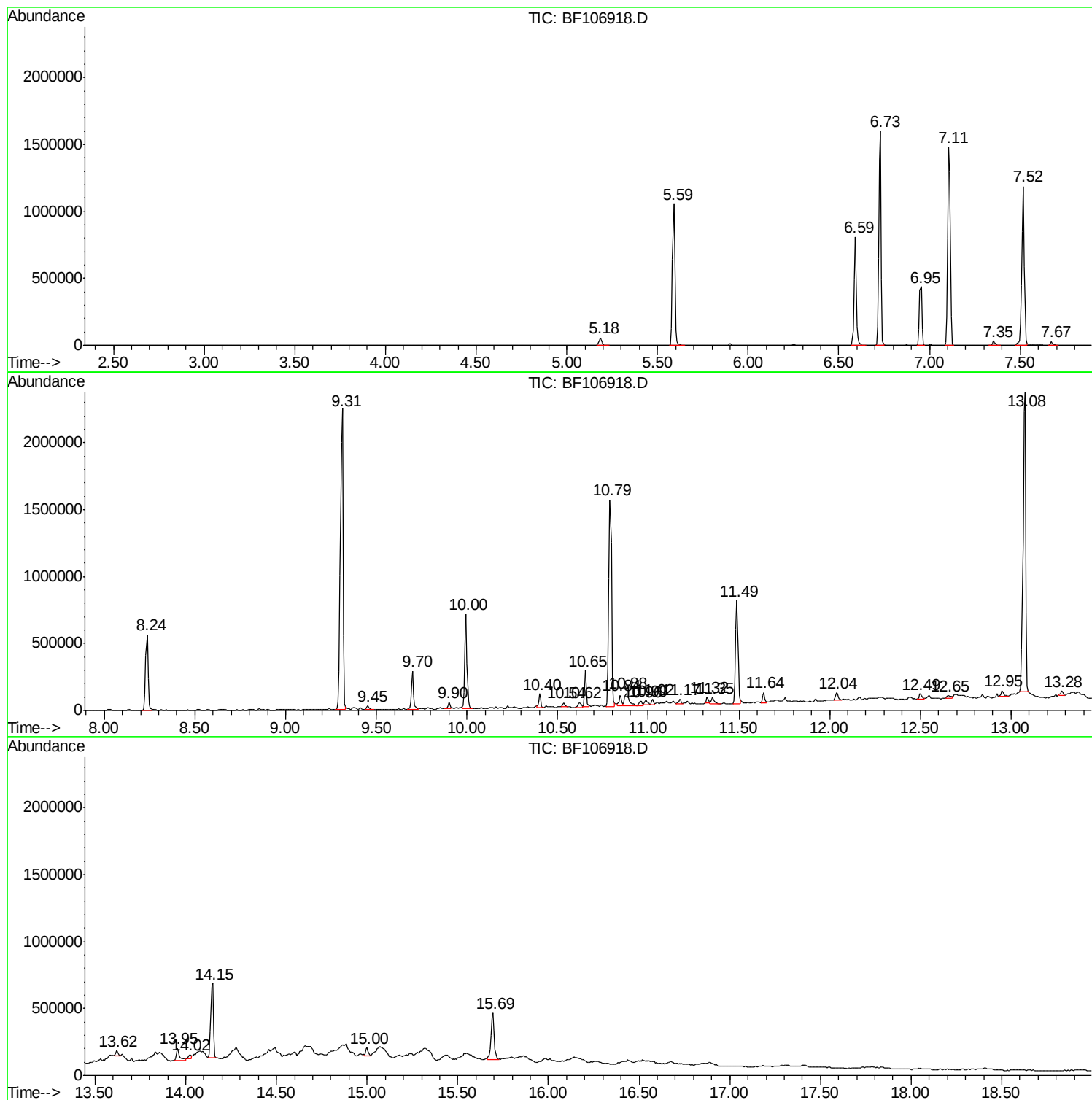
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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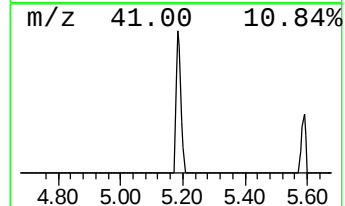
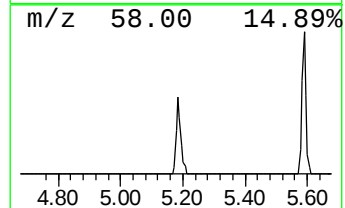
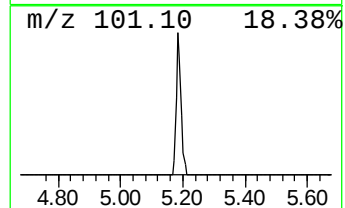
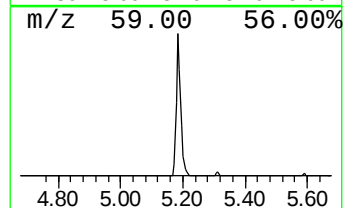
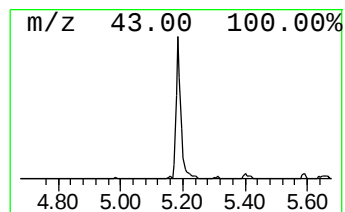
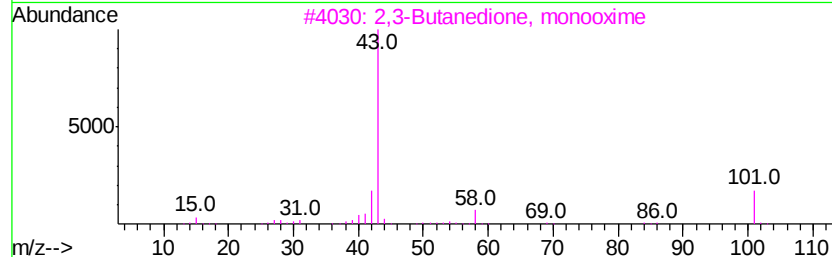
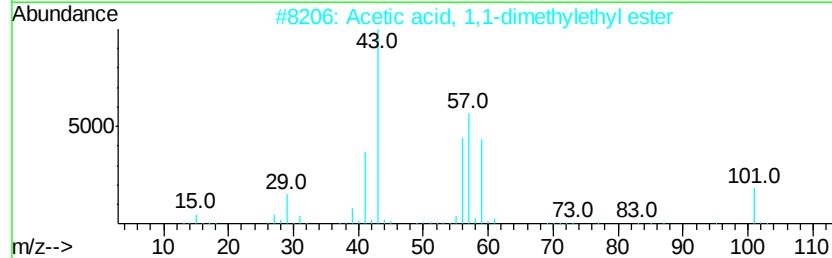
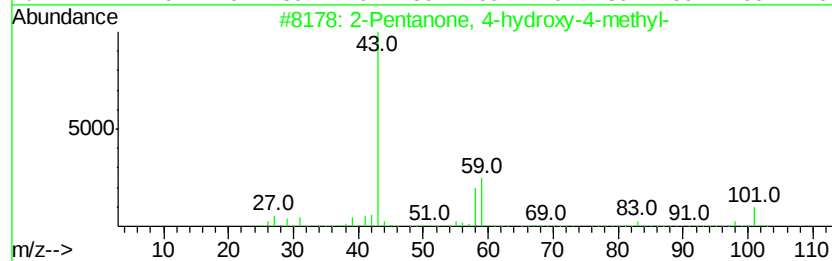
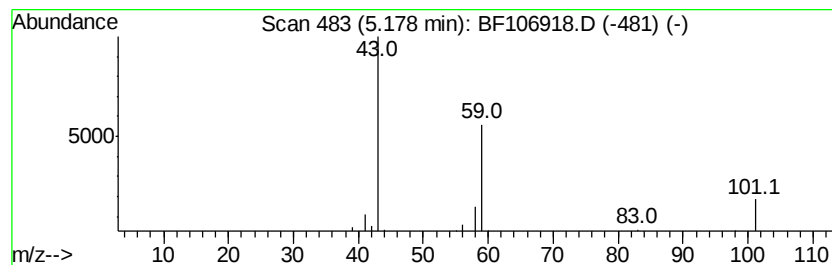
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.18	3.04 ng	59335	1,4-Dichlorobenzene-d4	6.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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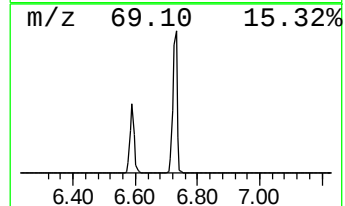
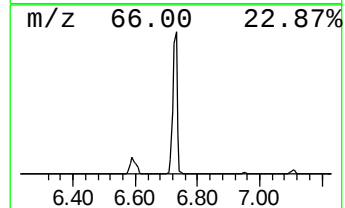
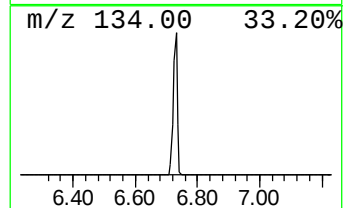
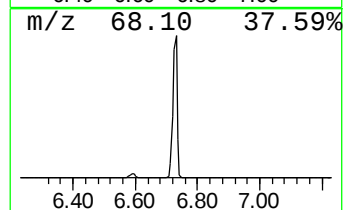
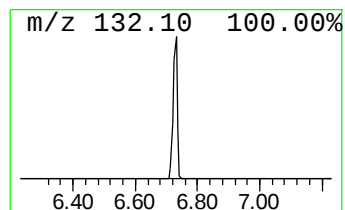
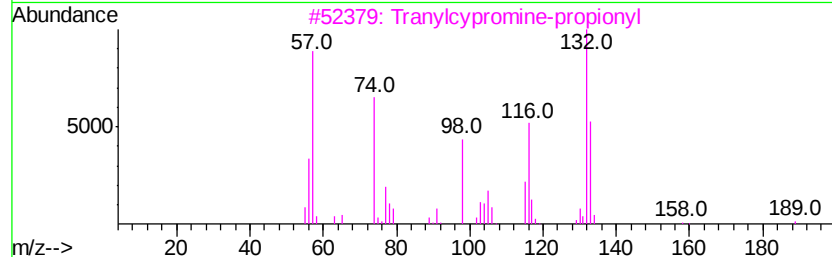
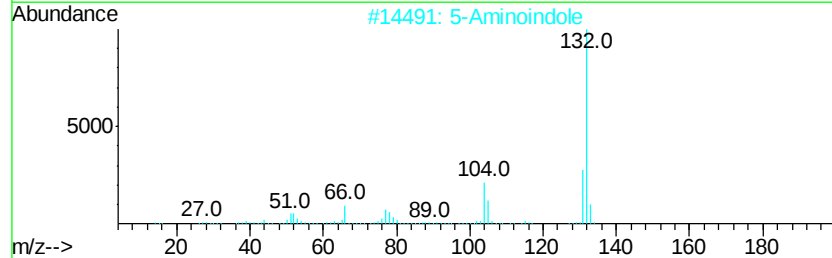
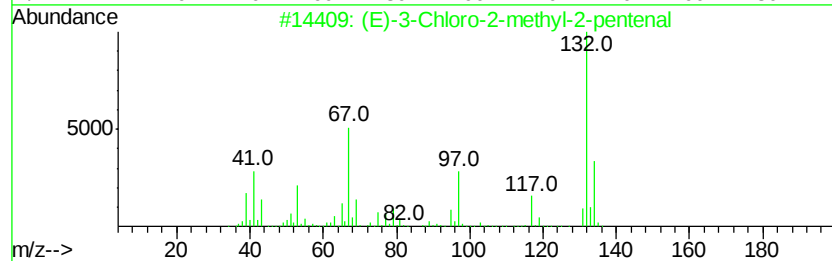
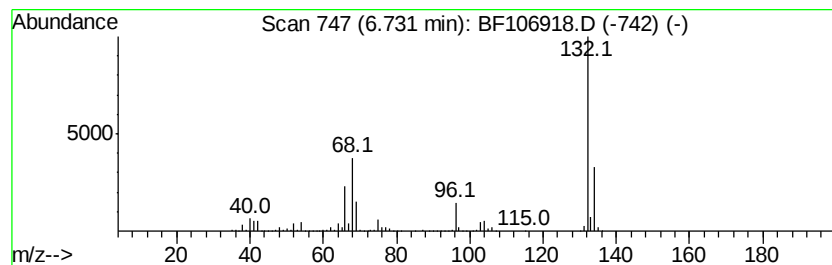
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	77.81 ng	1520380	1,4-Dichlorobenzene-d4	6.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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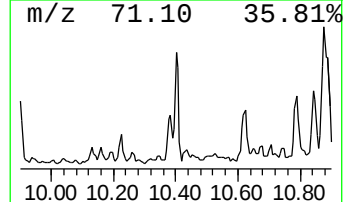
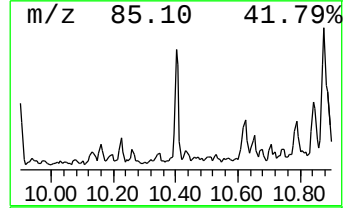
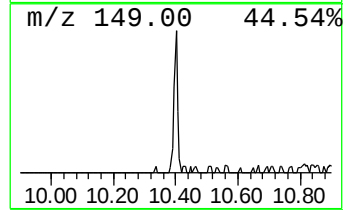
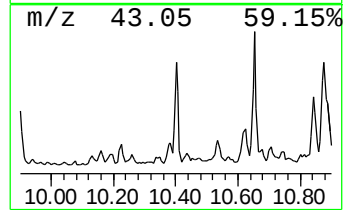
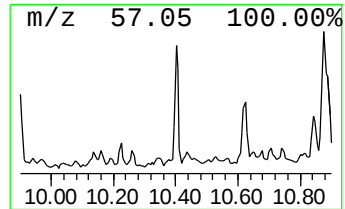
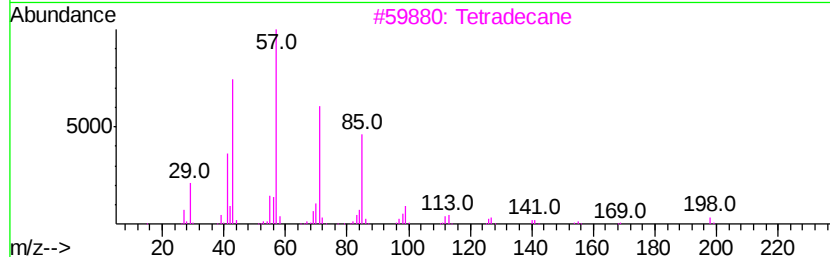
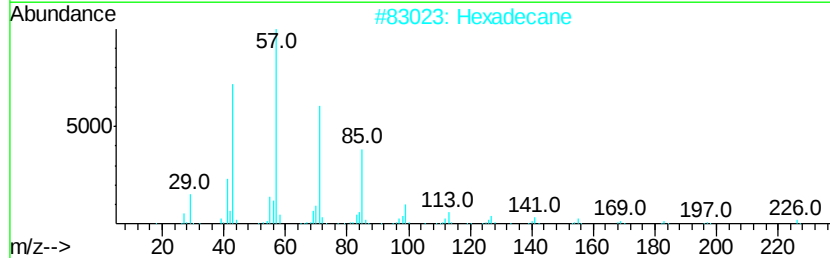
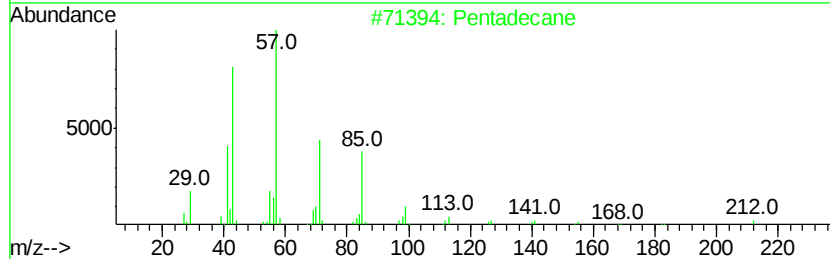
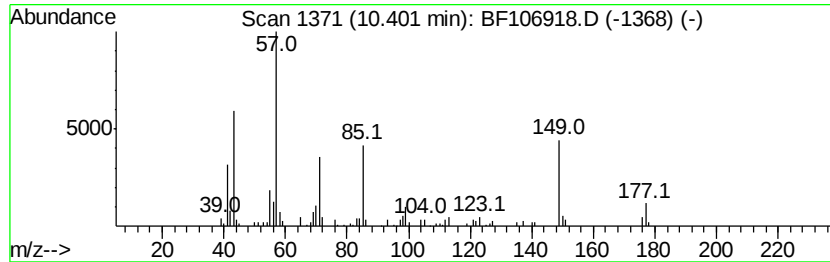
Instrument :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown10.40 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.40	2.83 ng	85841	Acenaphthene-d10		10.00
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	30
2	Hexadecane	226	C16H34	000544-76-3	27
3	Tetradecane	198	C14H30	000629-59-4	25
4	Heptadecane	240	C17H36	000629-78-7	25
5	Tridecane, 2,5-dimethyl-	212	C15H32	056292-66-1	22



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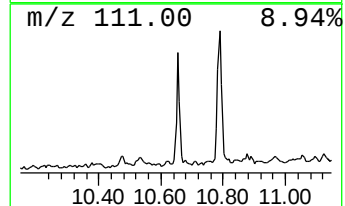
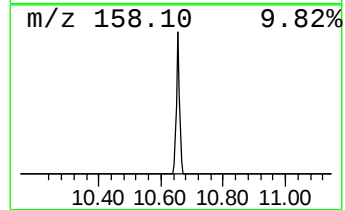
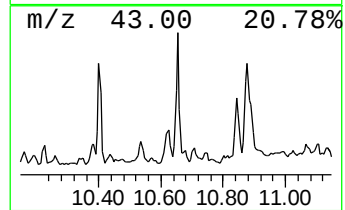
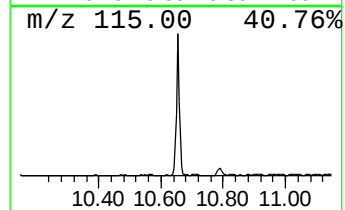
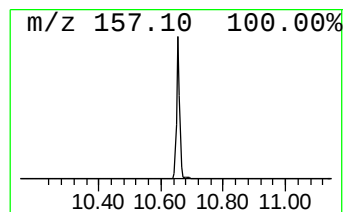
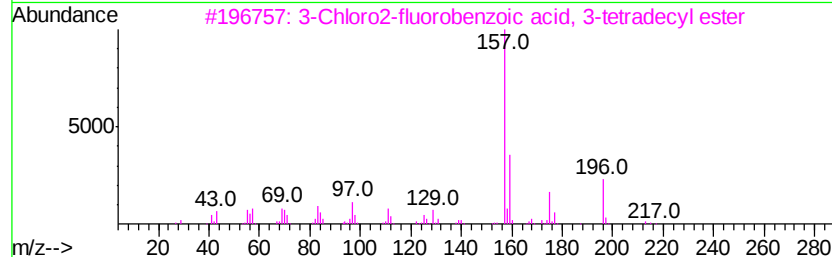
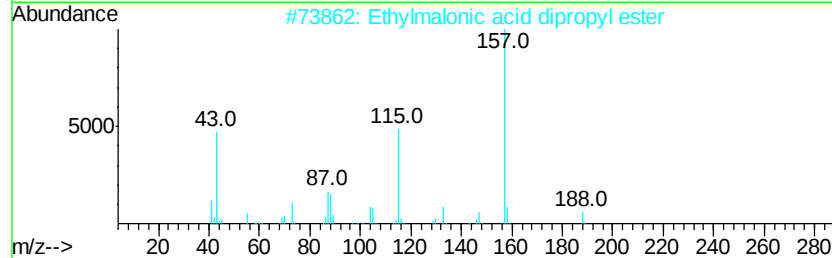
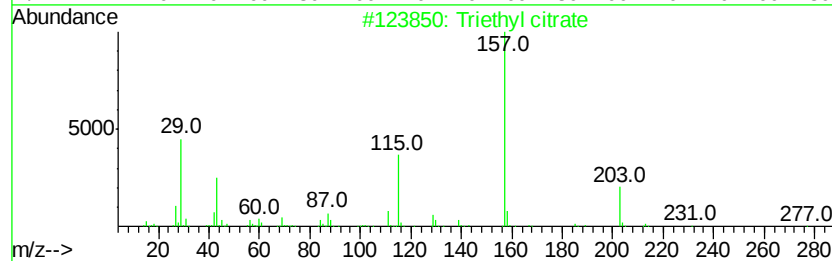
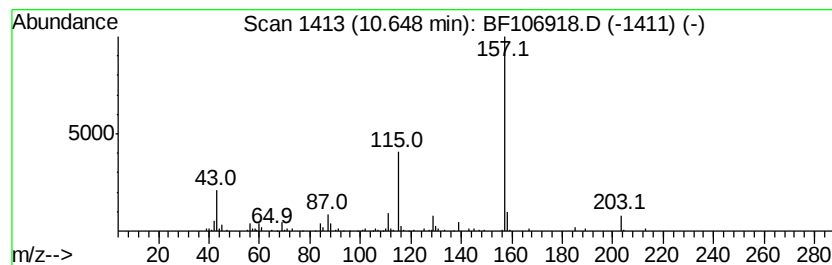
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Triethyl citrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.65	6.65 ng	201260	Acenaphthene-d10	10.00
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Triethyl citrate	276 C12H20O7	000077-93-0 83
2		Ethylmalonic acid dipropyl ester	216 C11H20O4	001113-91-3 59
3		3-Chloro2-fluorobenzoic acid, 3-...	370 C21H32ClF02	1000338-64-6 36
4		Piperazine-1-carboxylic acid, 4-...	362 C14H19ClN2O5S	1000303-80-2 36
5		1,4-Dioxaspiro[4.4]nonane, 7,8-b...	188 C9H16O4	1000155-54-9 33



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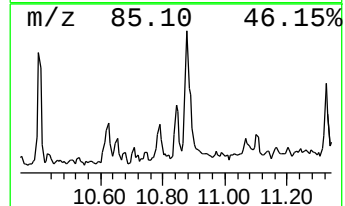
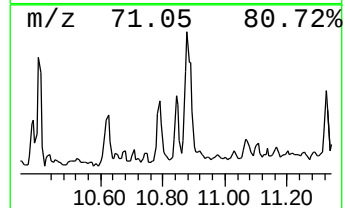
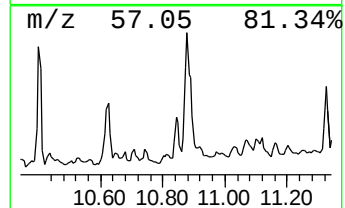
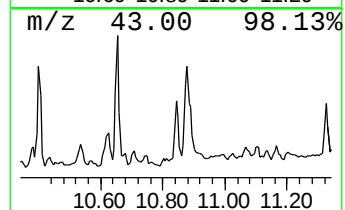
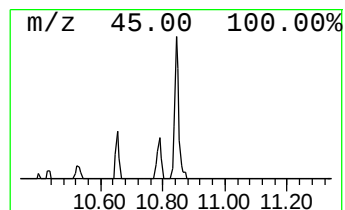
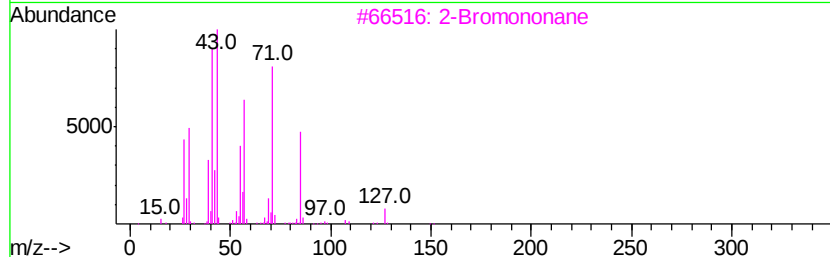
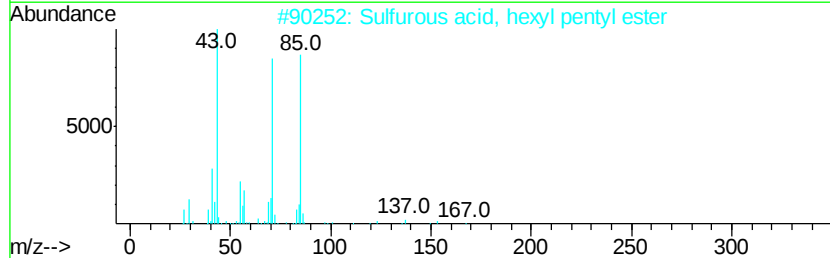
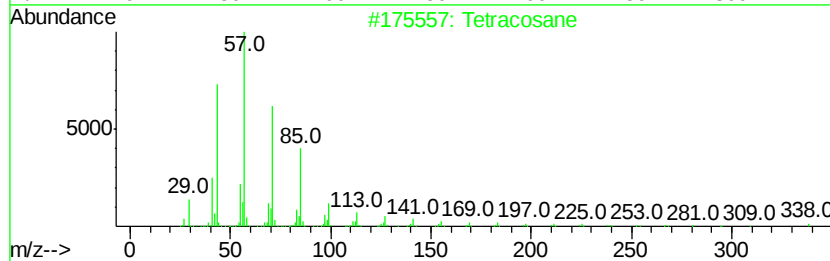
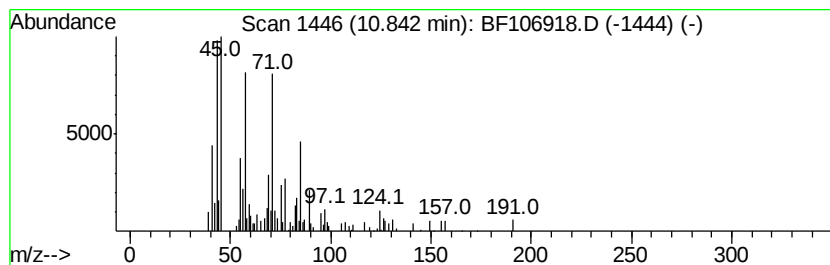
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown10.84 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.84	2.15 ng	72204	Phenanthrene-d10	11.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	35
2		Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	27
3		2-Bromononane	206	C9H19Br	002216-35-5	27
4		Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	27
5		Nonane, 5-butyl-	184	C13H28	017312-63-9	27



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062818\
Data File : BF106918.D
Acq On : 28 Jun 2018 14:10
Operator : JU/SJ
Sample : J3570-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

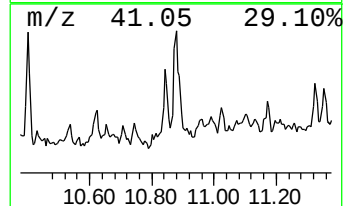
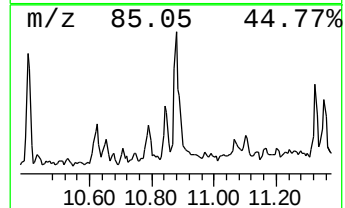
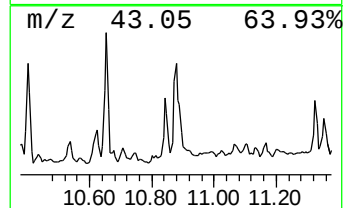
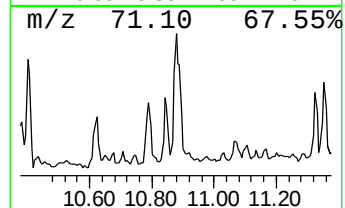
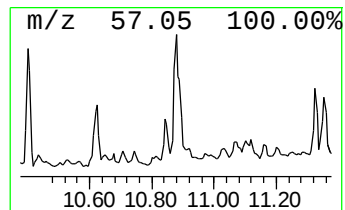
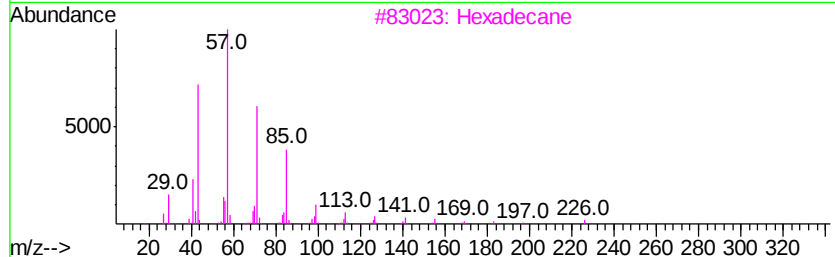
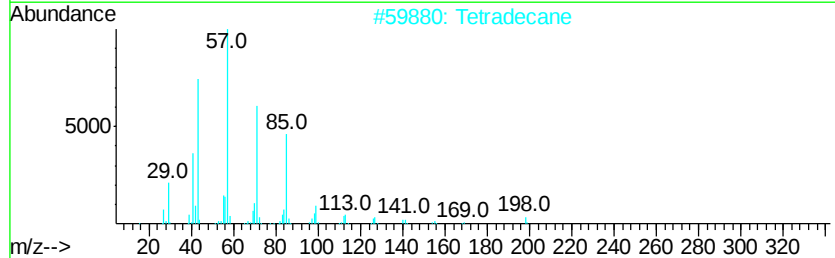
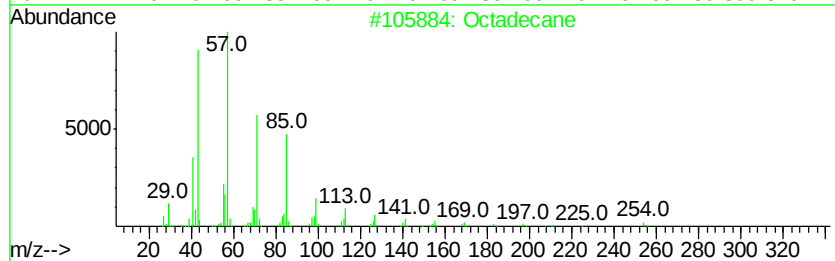
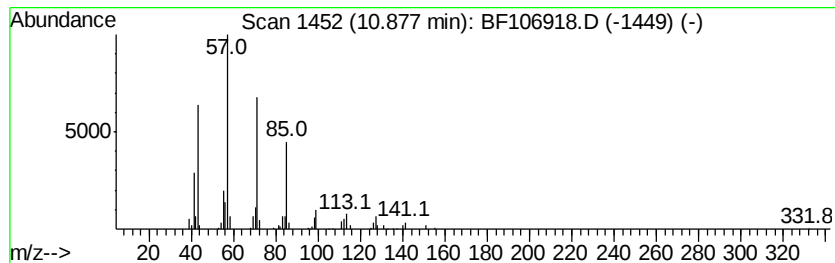
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ClientSampleId :
20180375-COMPOSITE-CS-1A-ELU

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.88	4.29 ng	143963	Phenanthrene-d10	11.49	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	90
2	Tetradecane	198	C14H30	000629-59-4	90
3	Hexadecane	226	C16H34	000544-76-3	90
4	Tridecane	184	C13H28	000629-50-5	90
5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062818\
Data File : BF106918.D
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Operator : JU/SJ
Sample : J3570-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

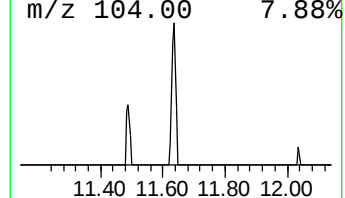
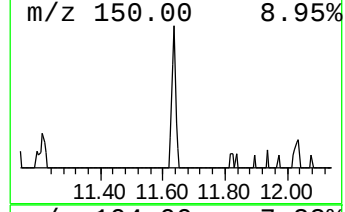
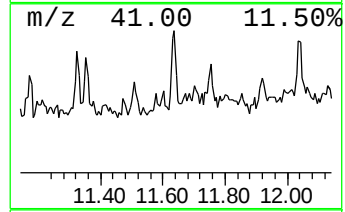
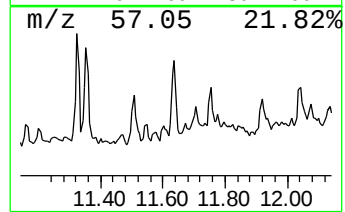
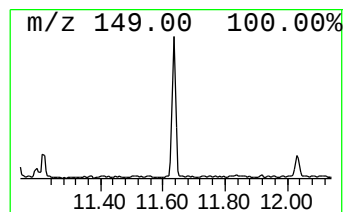
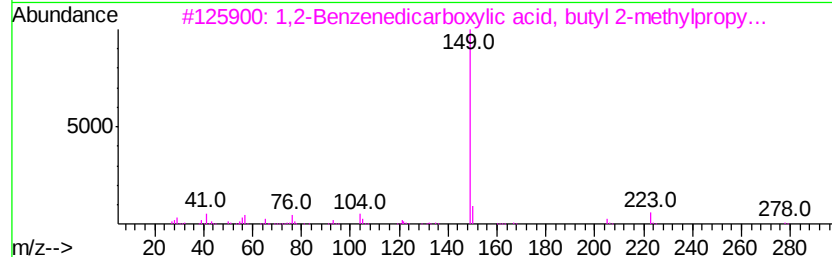
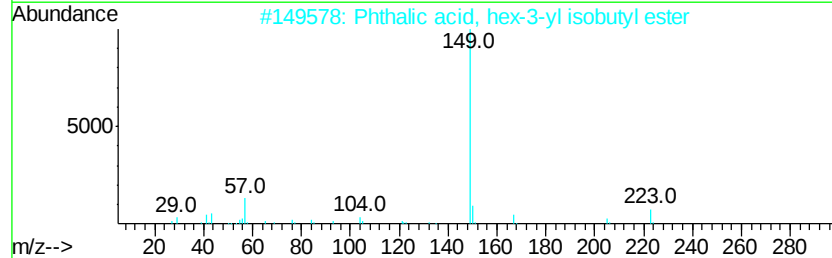
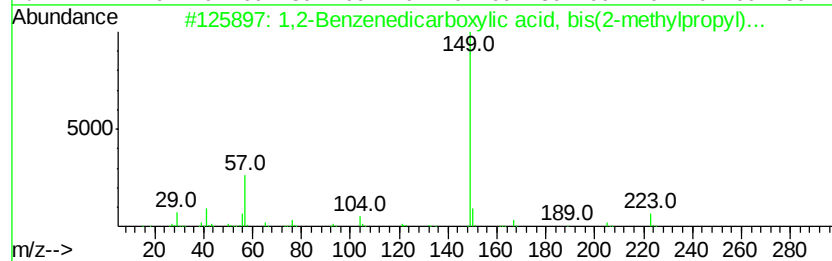
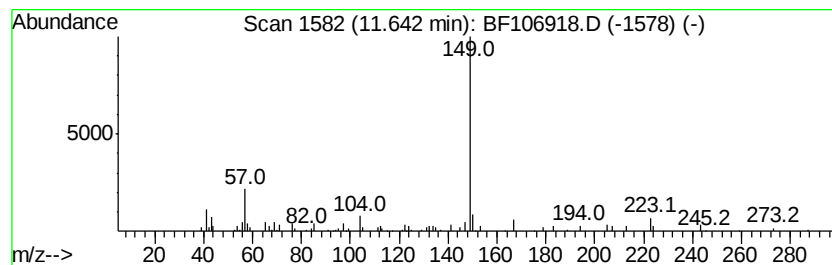
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1,2-Benzenedicarboxylic aci... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.		
11.64	2.08 ng	69954	Phenanthrene-d10		11.49		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Benzenedicarboxylic acid, bi...	278	C16H22O4	000084-69-5	90
2			Phthalic acid, hex-3-yl isobutyl...	306	C18H26O4	1000356-95-4	90
3			1,2-Benzenedicarboxylic acid, bu...	278	C16H22O4	017851-53-5	86
4			Phthalic acid, isobutyl octyl ester	334	C20H30O4	1000309-04-5	78
5			Phthalic acid, 2-ethoxyethyl pen...	308	C17H24O5	1000322-87-3	78



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062818\
Data File : BF106918.D
Acq On : 28 Jun 2018 14:10
Operator : JU/SJ
Sample : J3570-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

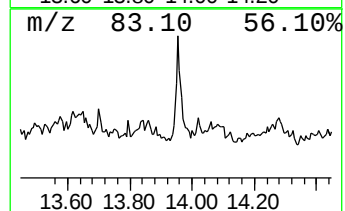
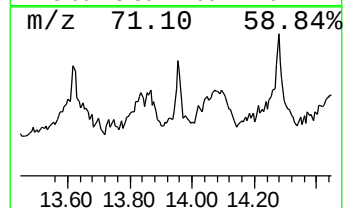
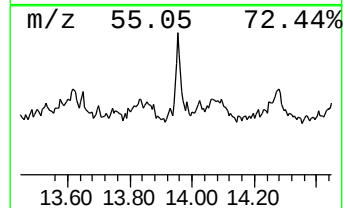
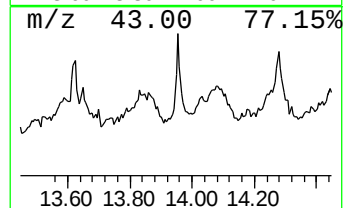
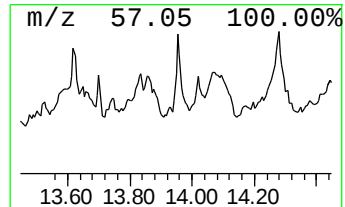
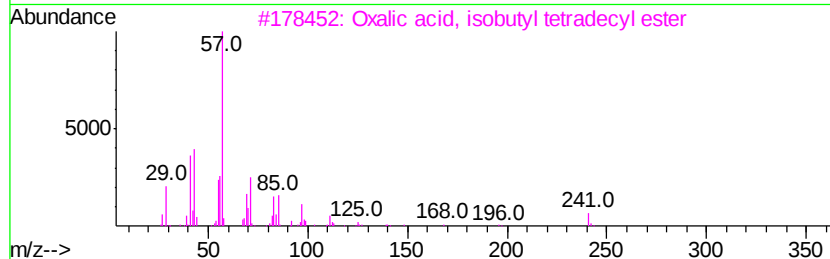
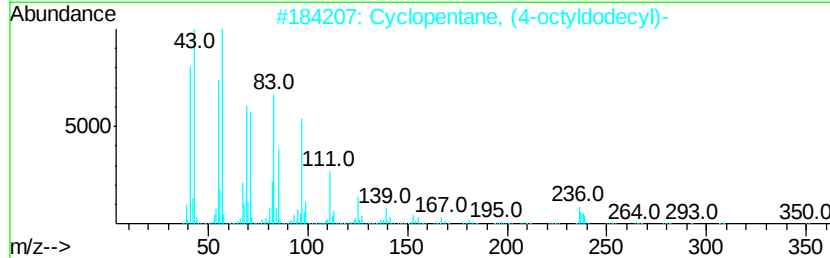
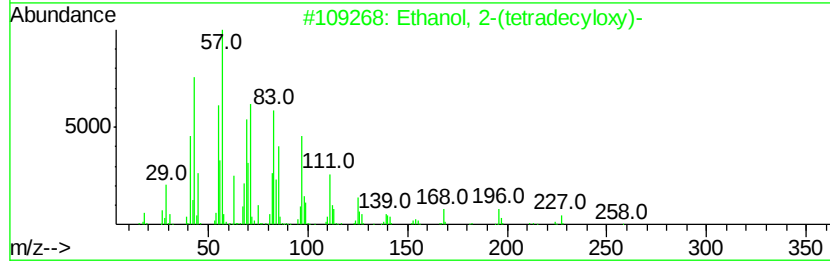
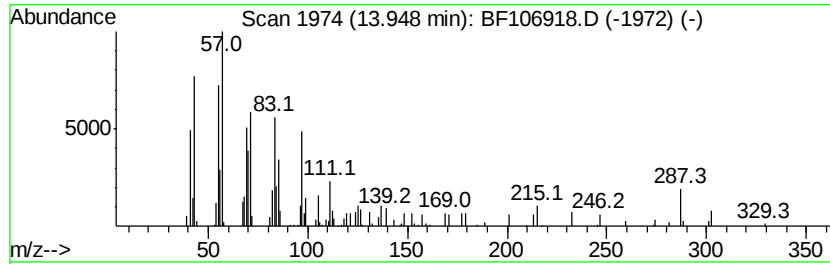
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Ethanol, 2-(tetradecyloxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.95	5.02 ng	134537	Chrysene-d12		14.15	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
2		Cyclopentane, (4-octyldodecyl)-	350	C25H50	005638-09-5	83
3		Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	83
4		17-Pentatriacontene	491	C35H70	006971-40-0	74
5		Hexacosyl trifluoroacetate	478	C28H53F3O2	1000351-75-0	74



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062818\
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Acq On : 28 Jun 2018 14:10
Operator : JU/SJ
Sample : J3570-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20180375-COMPOSITE-CS-1A-ELU

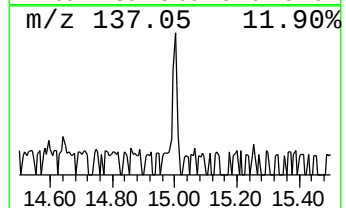
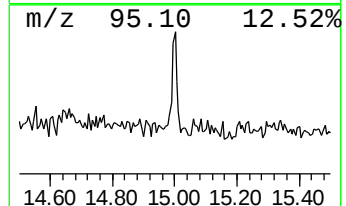
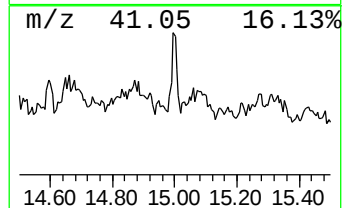
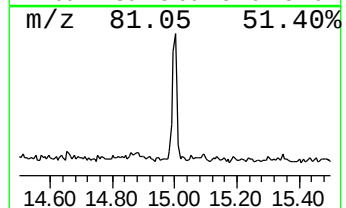
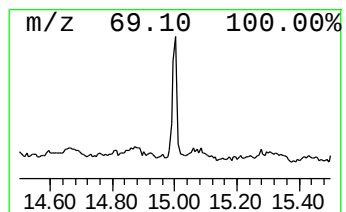
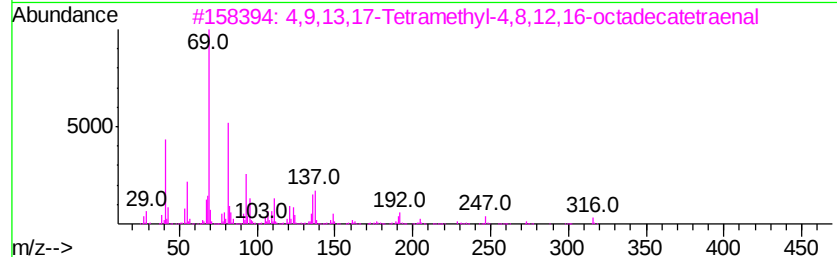
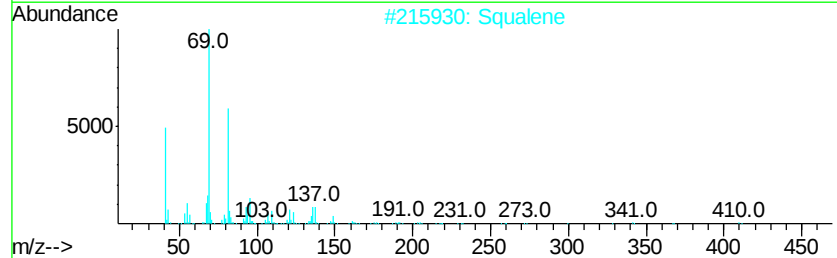
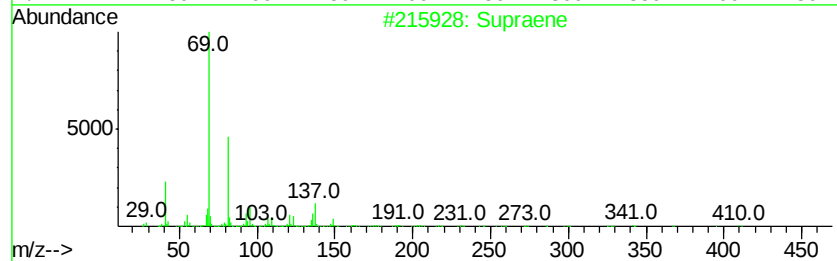
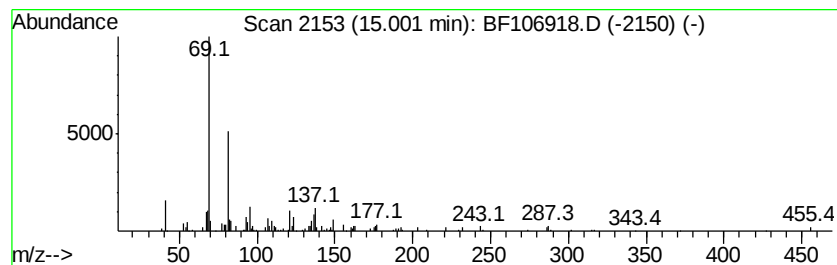
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Supraene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.00	2.64 ng	58496	Perylene-d12	15.69

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	90
2			Squalene	410	C30H50	000111-02-4	87
3			4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	78
4			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
5			1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF062818\
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Acq On : 28 Jun 2018 14:10
Operator : JU/SJ
Sample : J3570-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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...	5.18	3.0	ng	59335	1	6.95	390800	20.0
unknown6.73	6.73	77.8	ng	1520380	1	6.95	390800	20.0
unknown10.40	10.40	2.8	ng	85841	3	10.00	605747	20.0
Triethyl citrate	10.65	6.7	ng	201260	3	10.00	605747	20.0
unknown10.84	10.84	2.1	ng	72204	4	11.49	671375	20.0
Octadecane	10.88	4.3	ng	143963	4	11.49	671375	20.0
1,2-Benzenedicarb...	11.64	2.1	ng	69954	4	11.49	671375	20.0
Ethanol, 2-(tetra...	13.95	5.0	ng	134537	5	14.15	535760	20.0
Supraene	15.00	2.6	ng	58496	6	15.69	442966	20.0