

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF090618\
 Data File : BF108842.D
 Acq On : 6 Sep 2018 23:52
 Operator : JU/SJ
 Sample : J4803-17
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EP1-Q2-J6

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-BF090518.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	4.931	437	441	451	rVB	127827	166348	4.30%	0.442%
2	5.342	507	511	515	rBV	3318226	3359939	86.95%	8.925%
3	6.366	680	685	688	rBV	3827077	3509083	90.81%	9.321%
4	6.501	704	708	712	rBV	3879952	3541853	91.65%	9.408%
5	6.566	717	719	725	rVB	86856	73849	1.91%	0.196%
6	6.736	744	748	751	rBV	1706157	1357730	35.13%	3.606%
7	6.889	770	774	778	rBV	3141217	2841921	73.54%	7.549%
8	7.289	838	842	845	rBV	2352249	2228069	57.66%	5.918%
9	8.013	961	965	969	rBV	1836233	1660174	42.96%	4.410%
10	9.089	1144	1148	1151	rBV	4401636	3864394	100.00%	10.265%
11	9.219	1167	1170	1173	rVB	48937	42844	1.11%	0.114%
12	9.483	1211	1215	1218	rBV	1457539	1083173	28.03%	2.877%
13	9.766	1259	1263	1267	rVB	1979173	1653852	42.80%	4.393%
14	10.542	1392	1395	1402	rBV	1770763	1689478	43.72%	4.488%
15	10.648	1410	1413	1416	rBV	191875	151057	3.91%	0.401%
16	11.242	1510	1514	1516	rBV	1642716	1414952	36.62%	3.758%
17	11.266	1516	1518	1521	rVB	80758	62174	1.61%	0.165%
18	11.777	1601	1605	1609	rBV2	101211	113881	2.95%	0.302%
19	12.442	1715	1718	1722	rBV	110944	99135	2.57%	0.263%
20	12.671	1752	1757	1760	rBV	132979	129633	3.35%	0.344%
21	12.824	1779	1783	1786	rBV	3417792	3003726	77.73%	7.978%
22	13.736	1935	1938	1945	rBV	160835	231168	5.98%	0.614%
23	13.865	1955	1960	1963	rBV	1878281	1662609	43.02%	4.416%
24	14.624	2087	2089	2092	rBV3	47791	48122	1.25%	0.128%
25	14.654	2092	2094	2099	rVB	114869	109644	2.84%	0.291%
26	14.724	2103	2106	2111	rVB	154627	146685	3.80%	0.390%
27	14.971	2145	2148	2152	rVB	196280	194458	5.03%	0.517%
28	15.271	2194	2199	2204	rBV	1505553	1722374	44.57%	4.575%
29	15.330	2205	2209	2215	rVB	247431	326569	8.45%	0.867%
30	15.742	2274	2279	2284	rBV	273265	403563	10.44%	1.072%
31	16.206	2353	2358	2364	rBV	256661	447181	11.57%	1.188%
32	16.759	2447	2452	2460	rBV	155983	308286	7.98%	0.819%

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Instrument :
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ClientSampleId :
EP1-Q2-J6

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

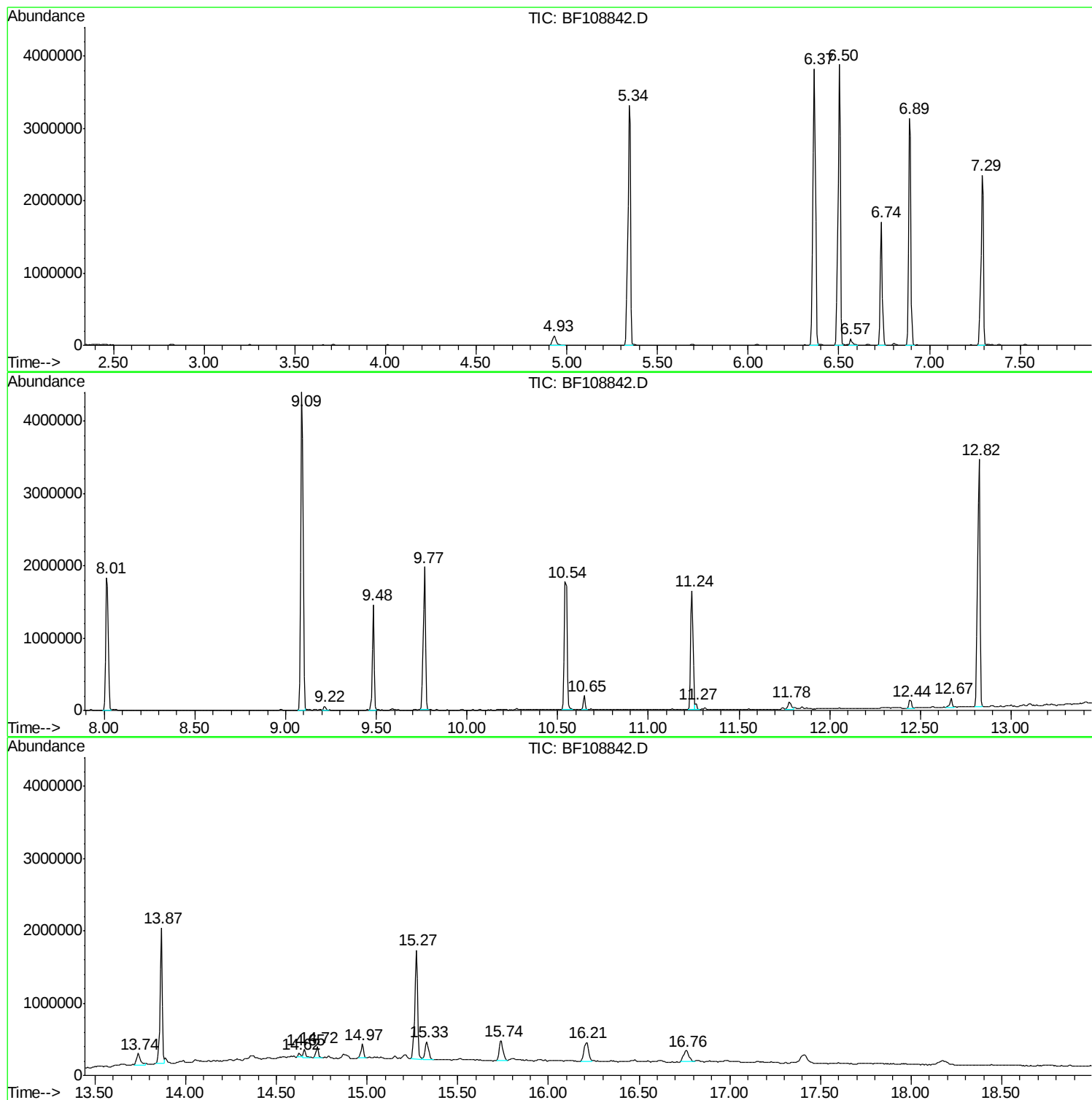
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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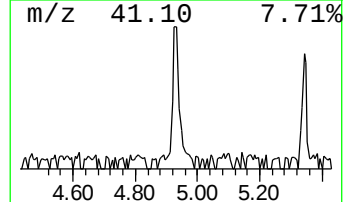
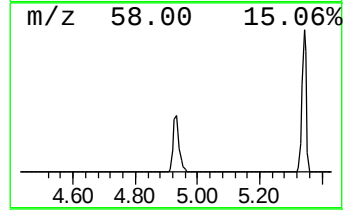
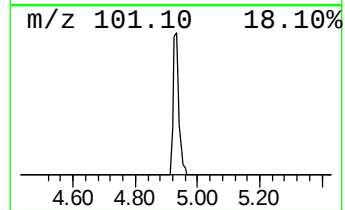
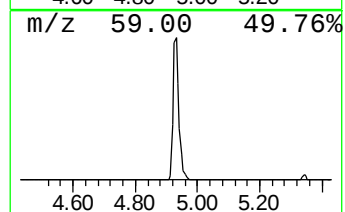
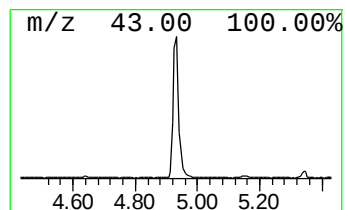
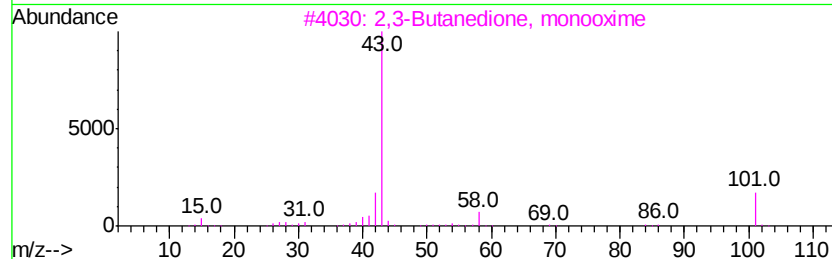
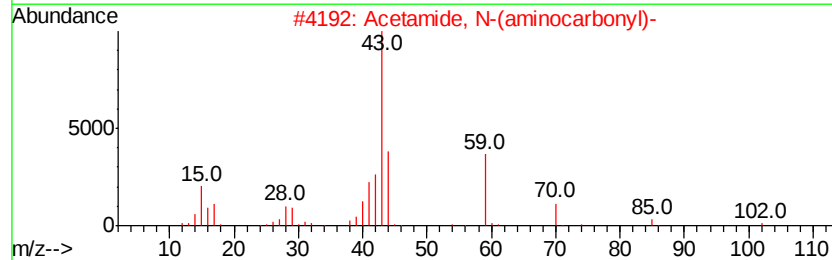
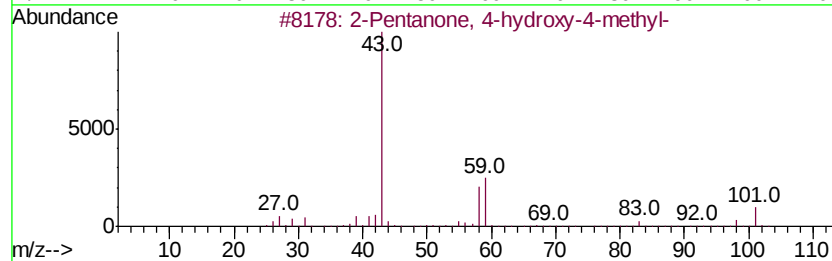
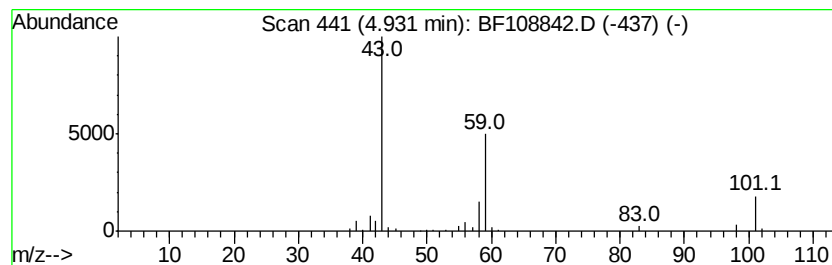
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	2.45 ng	166348	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetamide, N-(aminocarbonyl)-	102	C3H6N2O2	000591-07-1	9
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9



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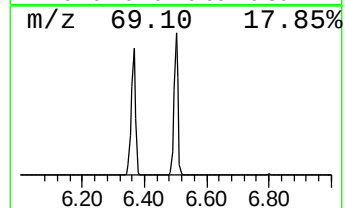
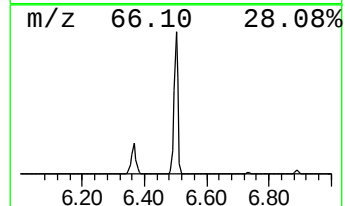
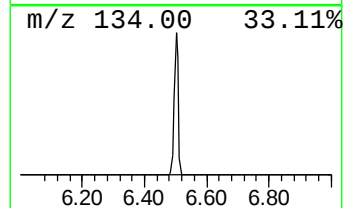
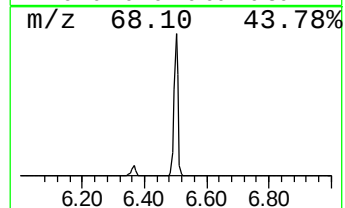
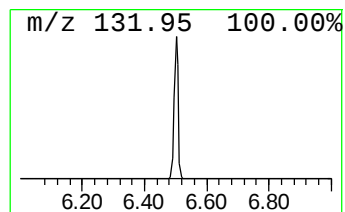
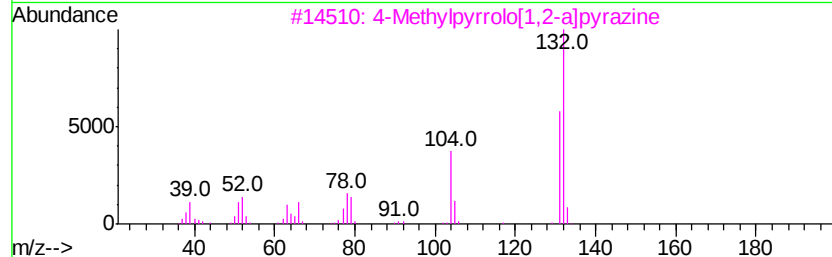
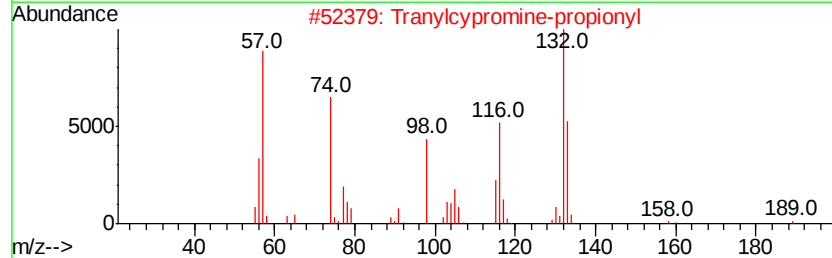
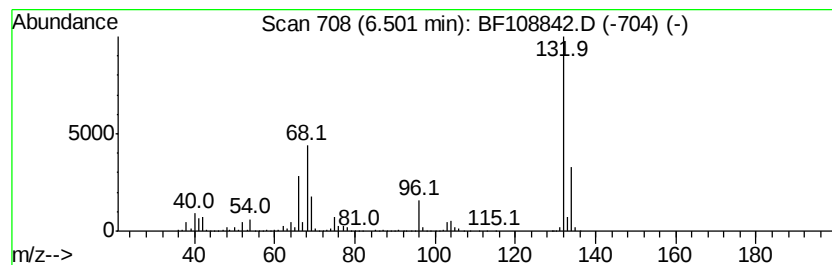
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF090518.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	52.17 ng	3541850	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10	
3	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9	
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9	
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9	



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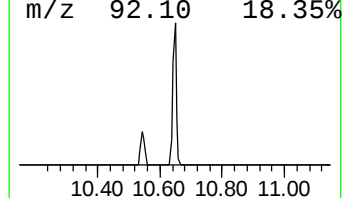
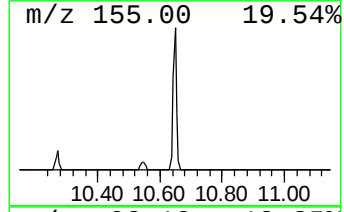
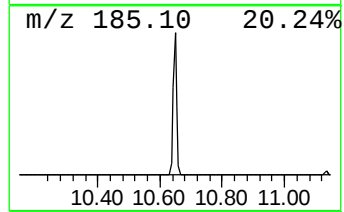
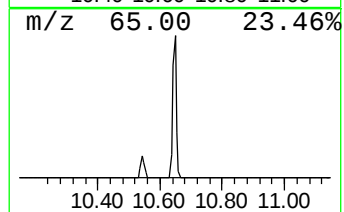
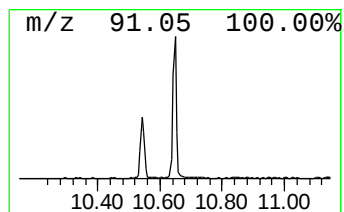
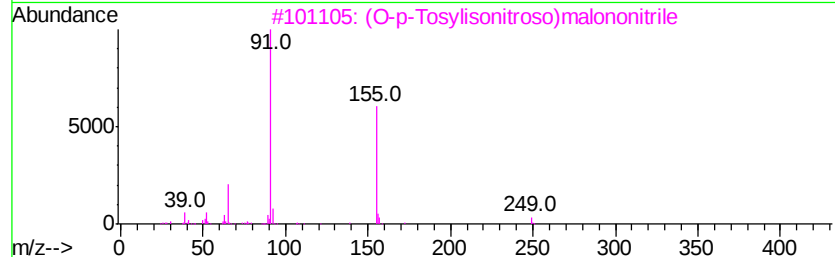
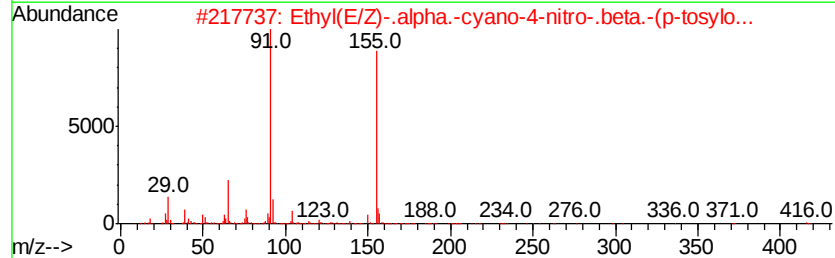
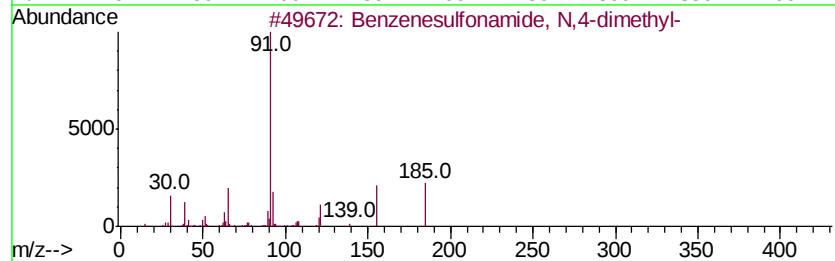
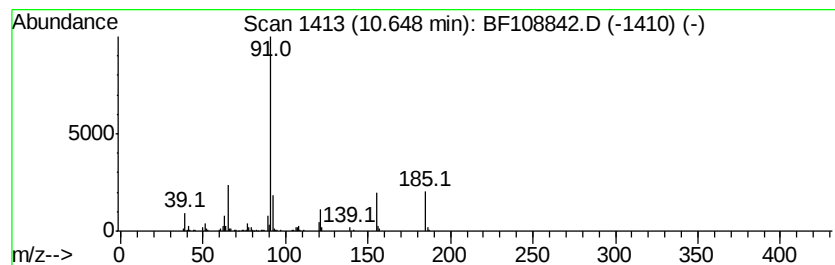
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzenesulfonamide, N,4-dim... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.65	2.14 ng	151057	Phenanthrene-d10	11.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	94
2		Ethyl(E/Z)-.alpha.-cyano-4-nitro...	416	C19H16N2O7S	1000287-26-8	53
3		(O-p-Tosylisonitroso)malononitrile	249	C10H7N3O3S	020893-01-0	47
4		Benzenesulfonamide, N,4-dimethyl...	214	C8H10N2O3S	000080-11-5	47
5		4-Toluenesulfonylmethyl isocyanide	195	C9H9NO2S	036635-61-7	47



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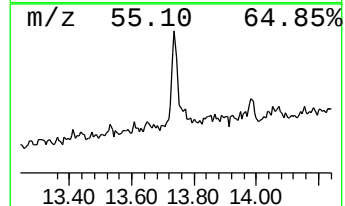
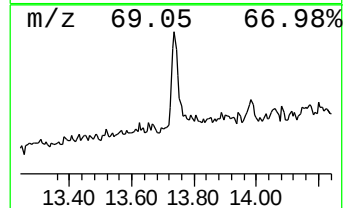
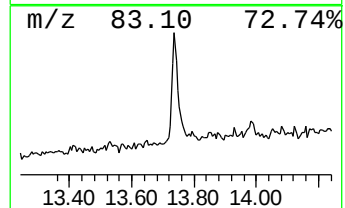
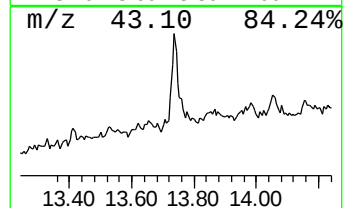
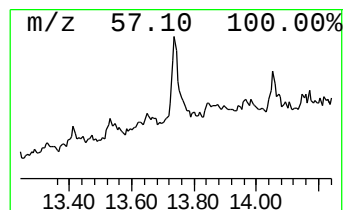
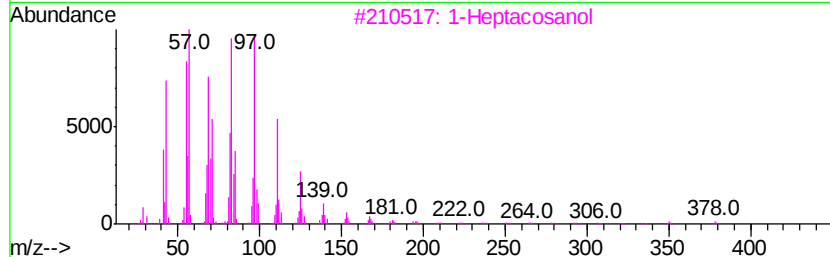
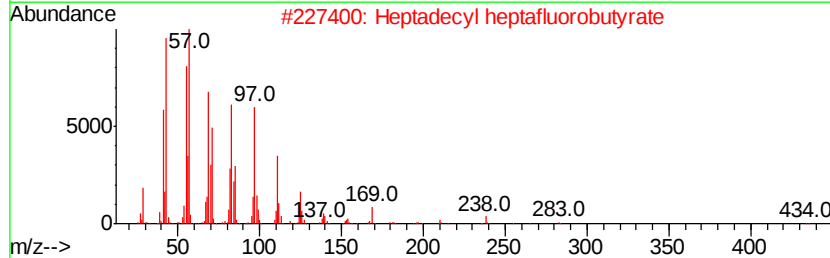
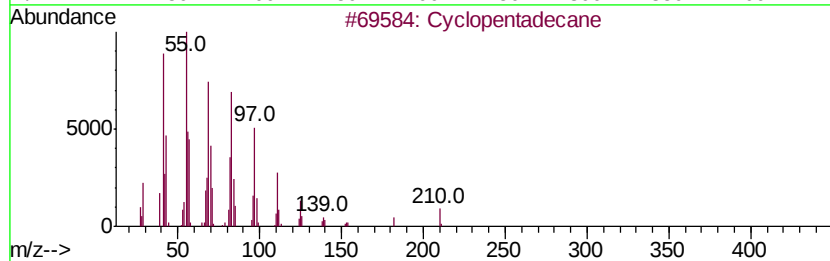
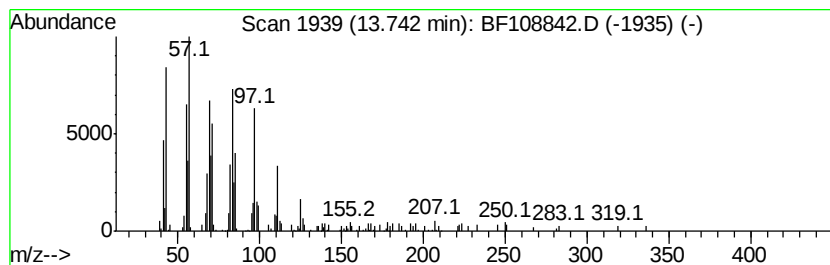
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Cyclopentadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	2.78 ng	231168	Chrysene-d12	13.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentadecane	210	C15H30	000295-48-7	95
2		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3		1-Heptacosanol	396	C27H56O	002004-39-9	91
4		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
5		2-Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91



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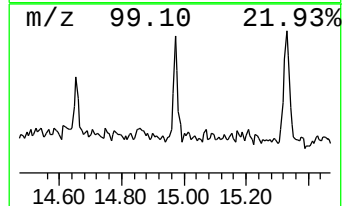
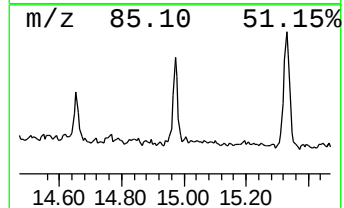
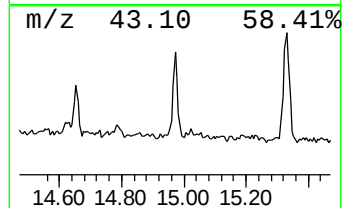
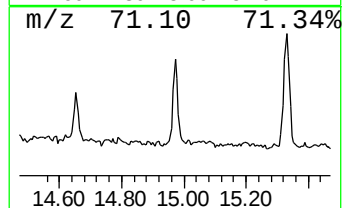
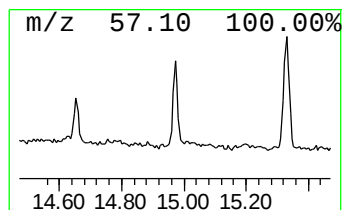
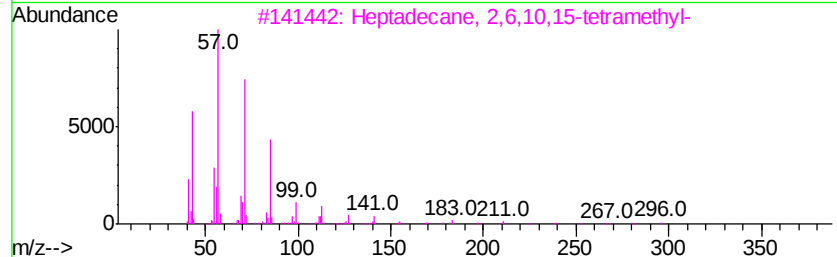
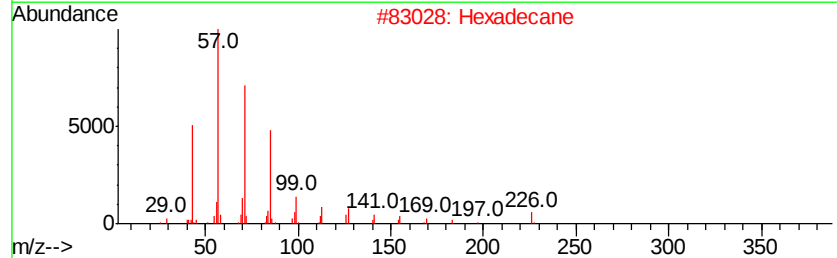
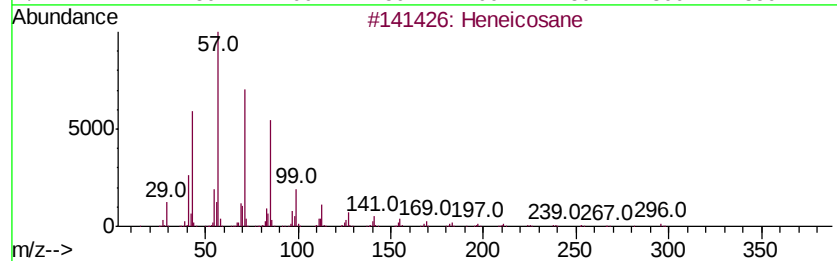
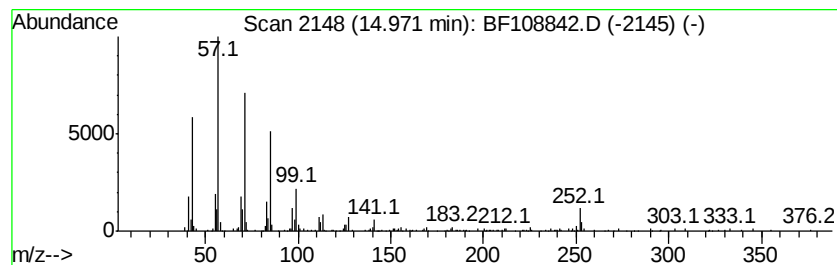
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.97	2.26 ng	194458	Perylene-d12	15.27

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	96
2	Hexadecane		226	C16H34	000544-76-3	93
3	Heptadecane, 2,6,10,15-tetramethyl-		296	C21H44	054833-48-6	93
4	Heptadecane		240	C17H36	000629-78-7	87
5	Hexacosane		366	C26H54	000630-01-3	81



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ClientSampleId :
EP1-Q2-J6

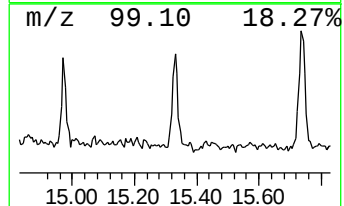
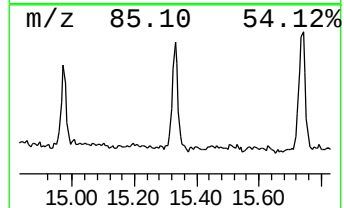
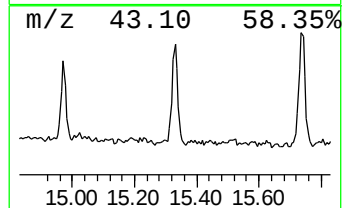
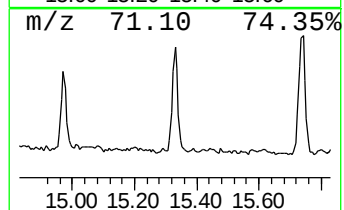
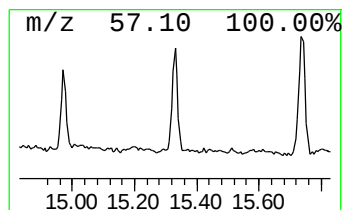
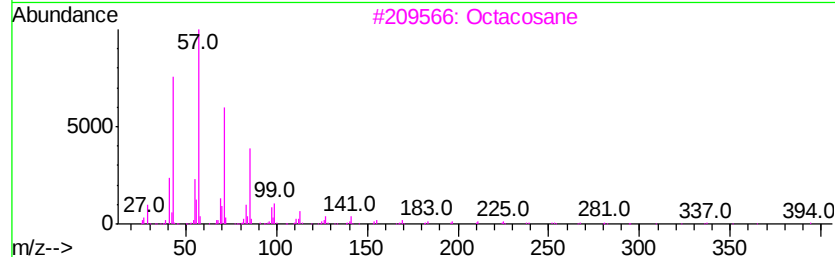
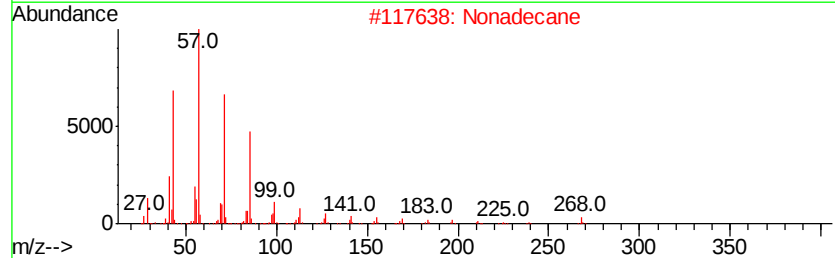
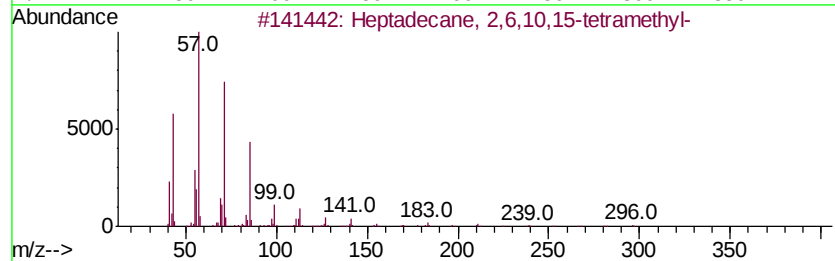
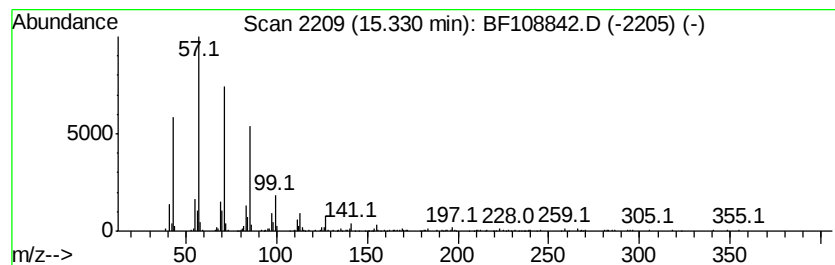
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecane, 2,6,10,15-tetr... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.33	3.79 ng	326569	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	94
2		Nonadecane	268	C19H40	000629-92-5	91
3		Octacosane	394	C28H58	000630-02-4	90
4		6,6-Diethylhoctadecane	310	C22H46	1000360-41-8	90
5		Heneicosane	296	C21H44	000629-94-7	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090618\
Data File : BF108842.D
Acq On : 6 Sep 2018 23:52
Operator : JU/SJ
Sample : J4803-17
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP1-Q2-J6

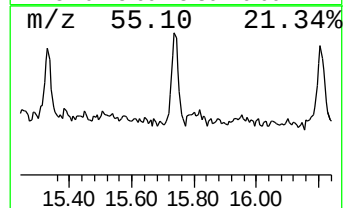
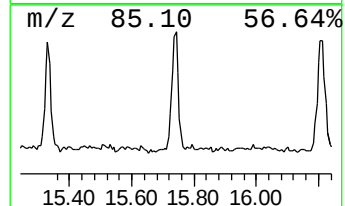
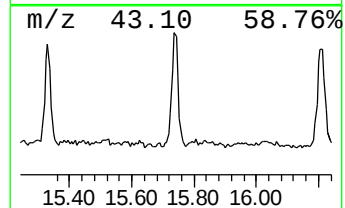
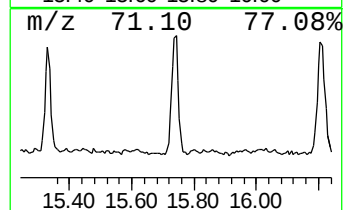
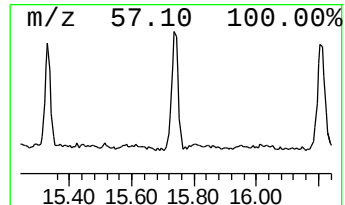
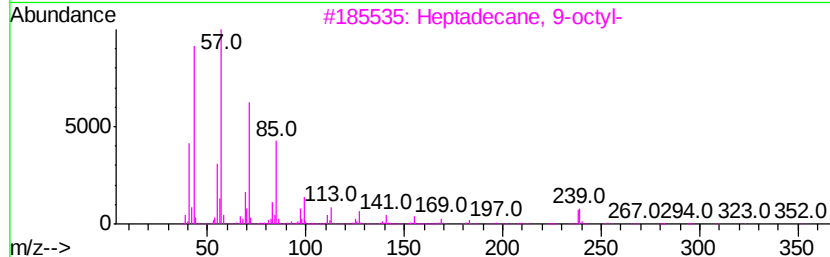
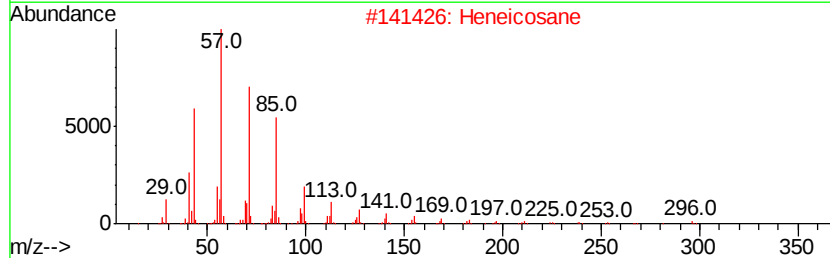
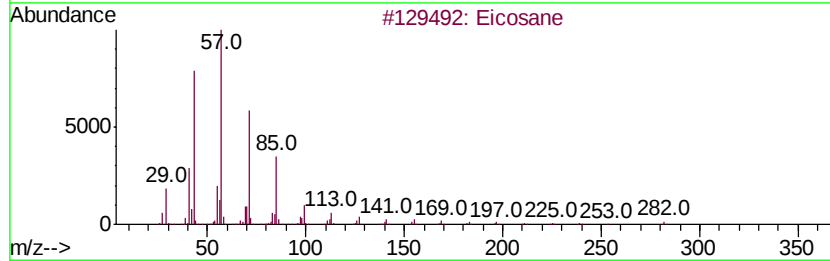
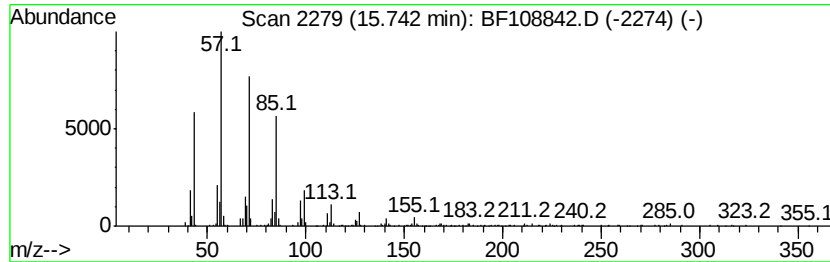
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.74	4.69 ng	403563	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4		Heptadecane	240	C17H36	000629-78-7	91
5		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090618\
 Data File : BF108842.D
 Acq On : 6 Sep 2018 23:52
 Operator : JU/SJ
 Sample : J4803-17
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EP1-Q2-J6

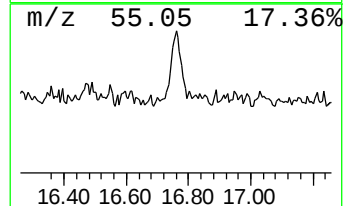
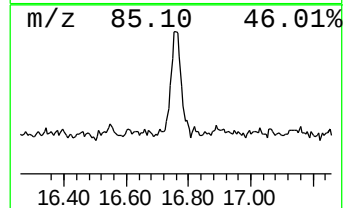
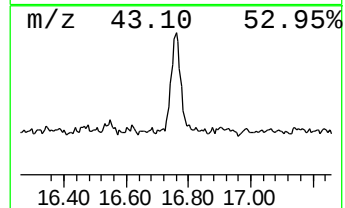
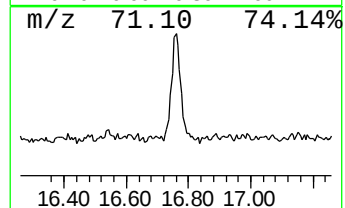
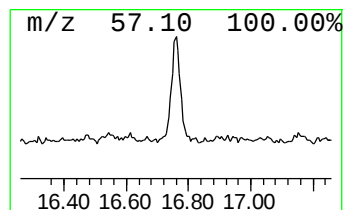
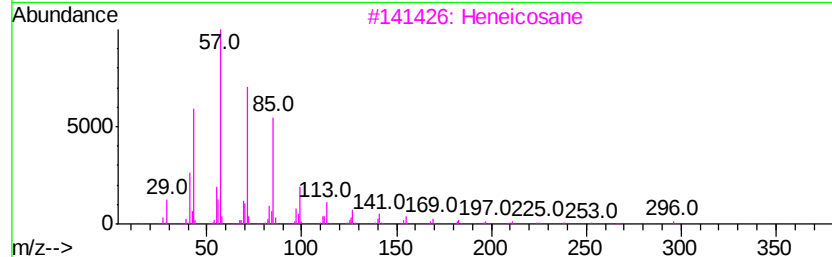
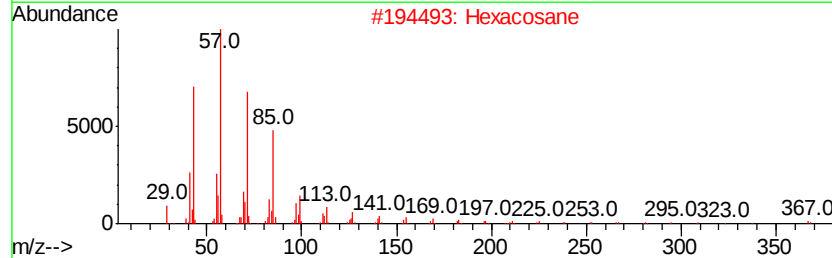
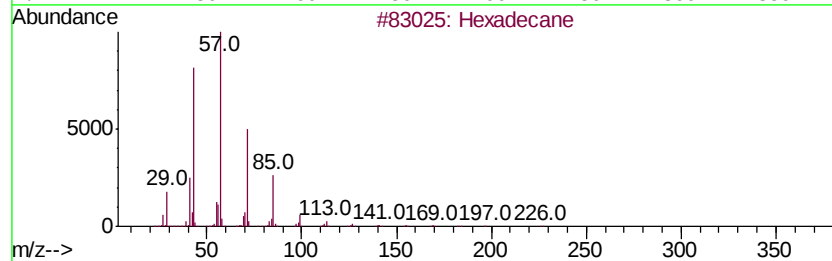
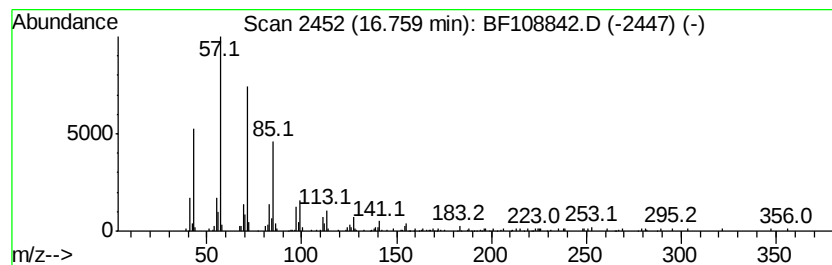
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 10 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.76	3.58 ng	308286	Perylene-d12	15.27

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	95
2			Hexacosane	366	C26H54	000630-01-3	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			Eicosane	282	C20H42	000112-95-8	91
5			2-methyloctacosane	408	C29H60	1000376-72-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF090618\
Data File : BF108842.D
Acq On : 6 Sep 2018 23:52
Operator : JU/SJ
Sample : J4803-17
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP1-Q2-J6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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...	4.93	2.5	ng	166348	1	6.74	1357730	20.0
unknown6.50	6.50	52.2	ng	3541850	1	6.74	1357730	20.0
Benzenesulfonamid...	10.65	2.1	ng	151057	4	11.24	1414950	20.0
Cyclopentadecane	13.74	2.8	ng	231168	5	13.87	1662610	20.0
Heneicosane	14.97	2.3	ng	194458	6	15.27	1722370	20.0
Heptadecane, 2,6,...	15.33	3.8	ng	326569	6	15.27	1722370	20.0
Eicosane	15.74	4.7	ng	403563	6	15.27	1722370	20.0
Hexadecane	16.76	3.6	ng	308286	6	15.27	1722370	20.0