

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
 Data File : BF107731.D
 Acq On : 27 Jul 2018 6:51
 Operator : JU/SJ
 Sample : J4142-05
 Misc :
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-1

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-BF072018.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	5.190	482	485	499	rBV	115884	175447	2.87%	0.443%
2	5.595	550	554	579	rBV	843369	1971940	32.31%	4.983%
3	6.595	721	724	744	rBV	688320	1576927	25.83%	3.985%
4	6.731	744	747	773	rVB	2901929	4133359	67.72%	10.445%
5	6.966	783	787	808	rVB	539186	1054086	17.27%	2.664%
6	7.113	808	812	838	rBV	3015433	3887805	63.69%	9.825%
7	7.525	878	882	894	rBV	1943135	2967833	48.62%	7.500%
8	7.678	905	908	915	rVB	130885	133056	2.18%	0.336%
9	8.242	1000	1004	1023	rBV	990836	1402641	22.98%	3.545%
10	9.319	1182	1187	1202	rBV	4676985	6104007	100.00%	15.425%
11	9.707	1249	1253	1260	rBV	216578	250062	4.10%	0.632%
12	10.001	1299	1303	1316	rBV	1384557	1513199	24.79%	3.824%
13	10.183	1329	1334	1339	rBV	54031	76001	1.25%	0.192%
14	10.278	1346	1350	1355	rBV	100244	101787	1.67%	0.257%
15	10.701	1417	1422	1430	rVB7	28676	68597	1.12%	0.173%
16	10.795	1434	1438	1463	rBV	2815832	3841770	62.94%	9.708%
17	11.377	1532	1537	1543	rBV2	89756	144831	2.37%	0.366%
18	11.495	1553	1557	1565	rBV	1105355	1411320	23.12%	3.566%
19	11.995	1634	1642	1654	rBV3	187828	378504	6.20%	0.956%
20	12.248	1682	1685	1688	rBV	129437	113042	1.85%	0.286%
21	12.501	1725	1728	1733	rBV	54960	73211	1.20%	0.185%
22	12.554	1733	1737	1743	rVV5	50606	81276	1.33%	0.205%
23	12.889	1789	1794	1798	rBV3	33135	61823	1.01%	0.156%
24	13.077	1821	1826	1848	rBV	3715531	4253426	69.68%	10.749%
25	13.283	1856	1861	1864	rBV	78264	64936	1.06%	0.164%
26	13.624	1916	1919	1922	rBV	153146	142735	2.34%	0.361%
27	13.954	1971	1975	1981	rBV	192785	204628	3.35%	0.517%
28	14.142	2003	2007	2020	rBV	921638	1147901	18.81%	2.901%
29	14.271	2026	2029	2033	rVB	150225	118573	1.94%	0.300%
30	14.577	2078	2081	2088	rVB	155584	143647	2.35%	0.363%
31	14.895	2132	2135	2141	rVB	150261	154823	2.54%	0.391%
32	14.977	2145	2149	2153	rVB	133460	133753	2.19%	0.338%
33	15.248	2191	2195	2200	rBV2	138932	156208	2.56%	0.395%
34	15.671	2259	2267	2280	rBV	683671	1240959	20.33%	3.136%

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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	16.107	2337	2341	2346	rVB	97158	146036	2.39%	0.369%
36	16.642	2427	2432	2438	rBV	76455	142006	2.33%	0.359%

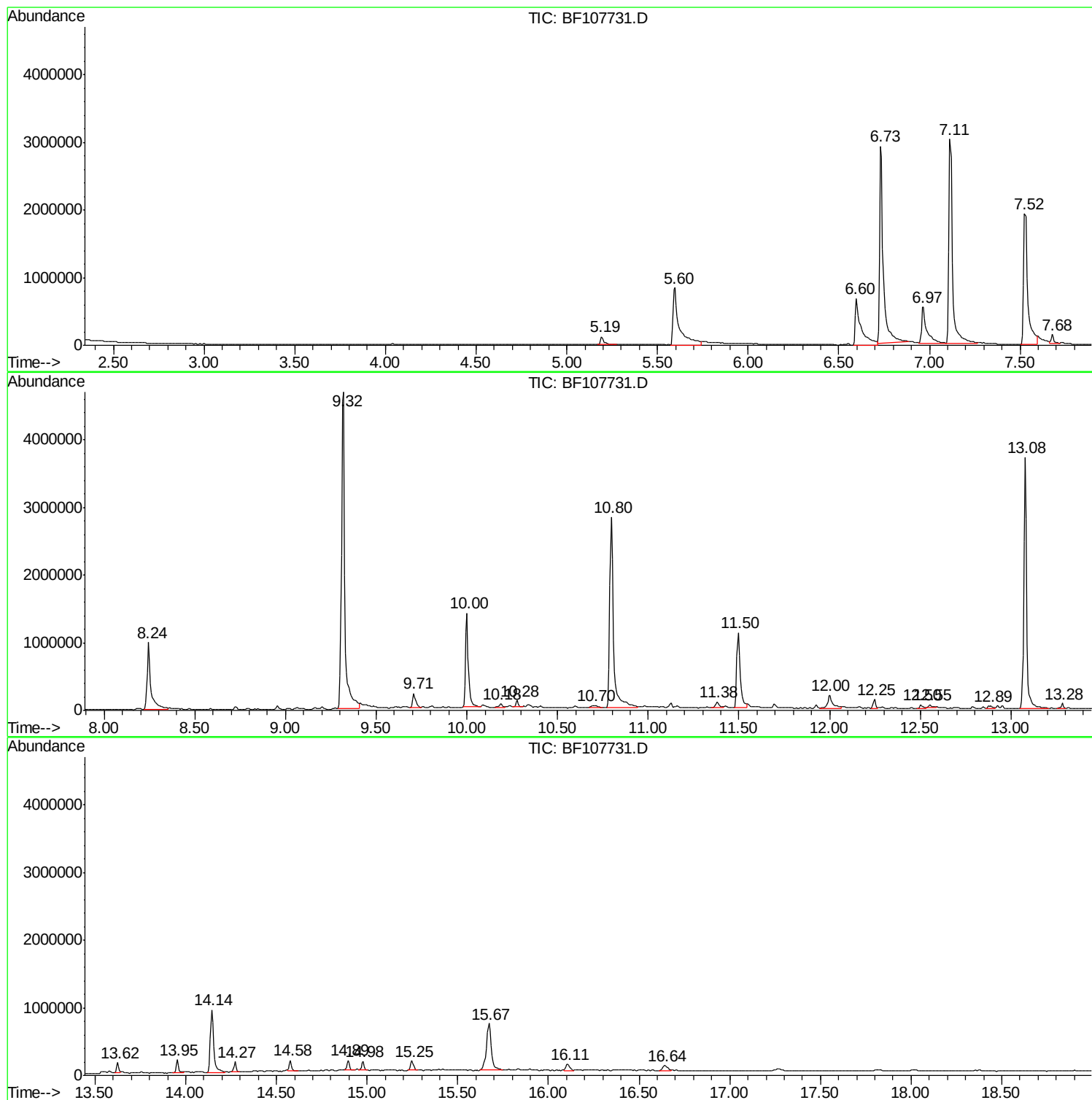
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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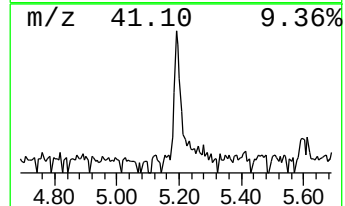
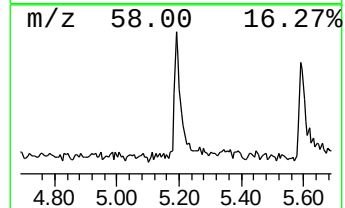
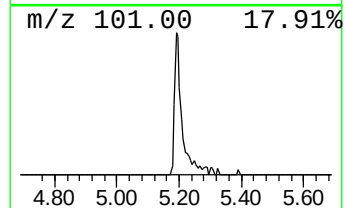
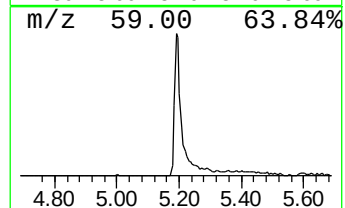
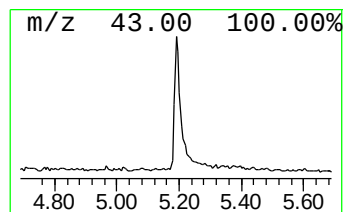
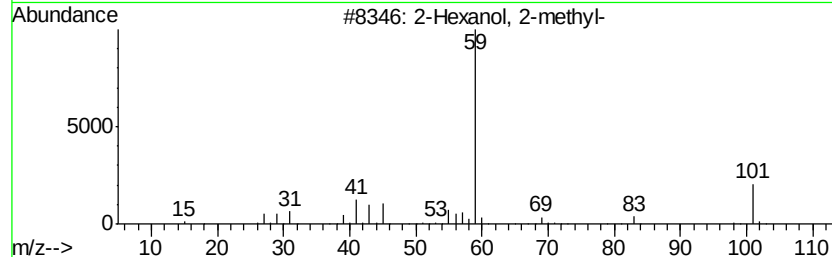
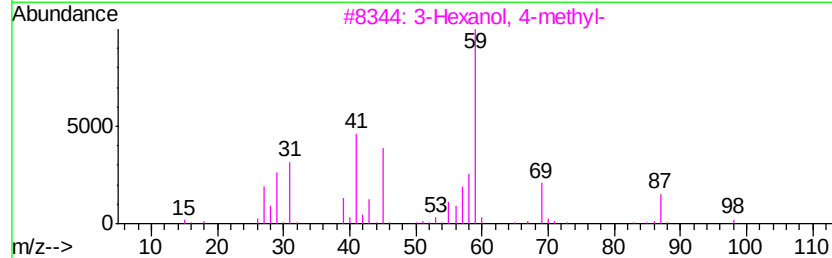
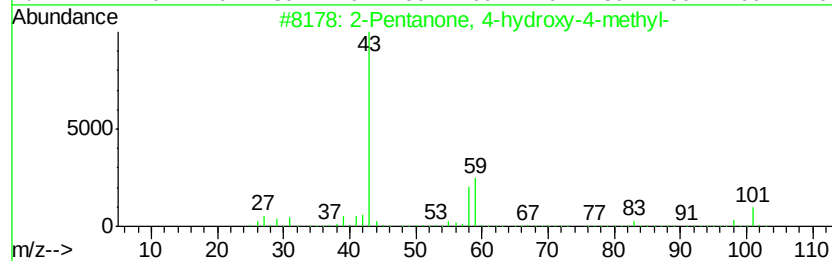
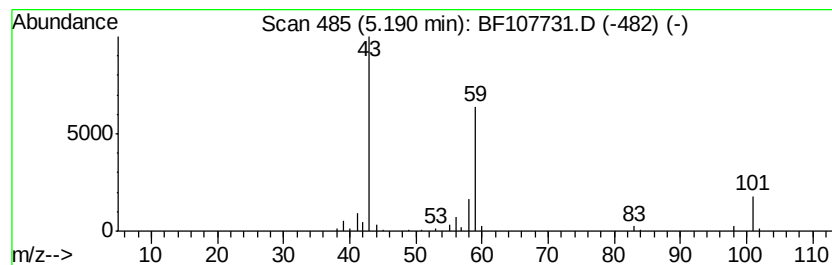
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	3.33 ng	175447	1,4-Dichlorobenzene-d4	6.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10



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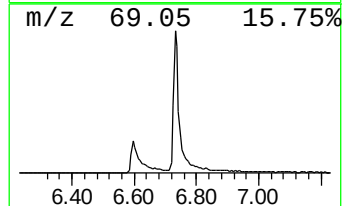
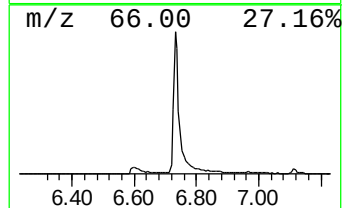
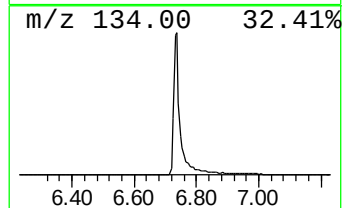
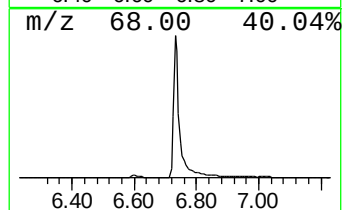
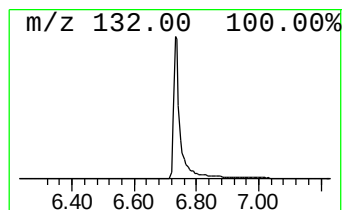
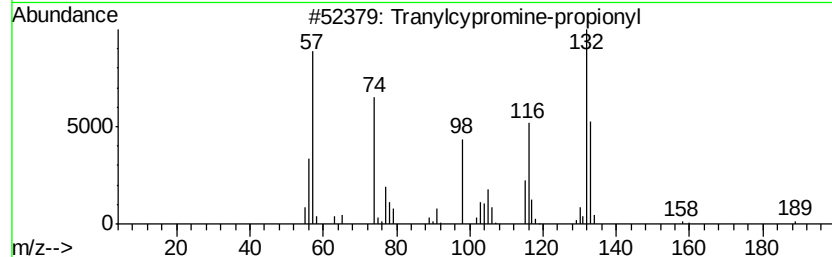
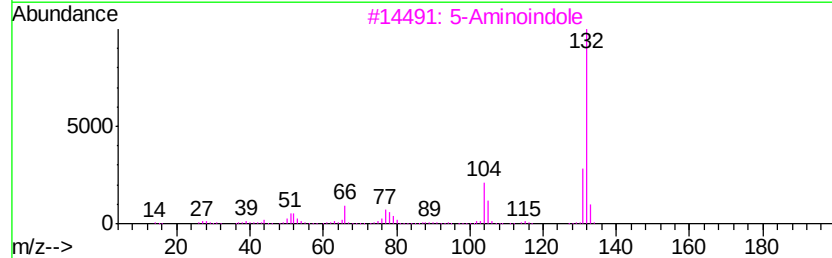
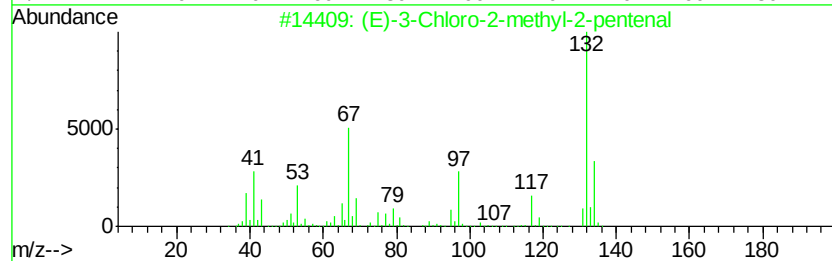
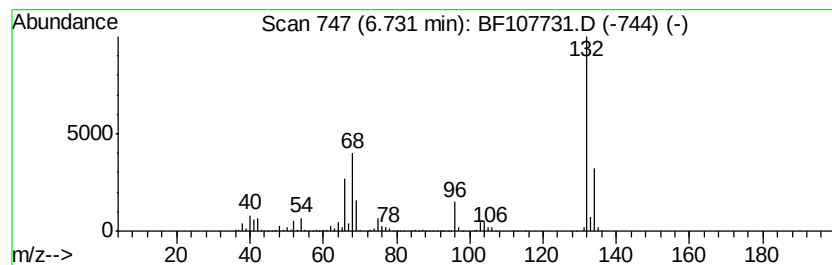
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	78.43 ng	4133360	1,4-Dichlorobenzene-d4	6.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5			4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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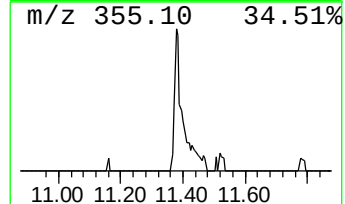
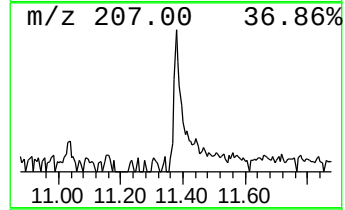
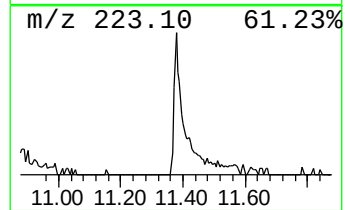
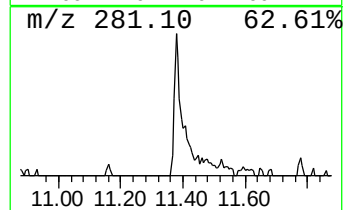
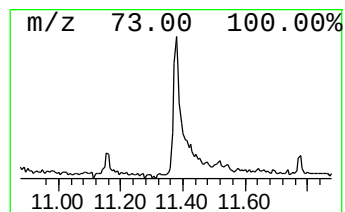
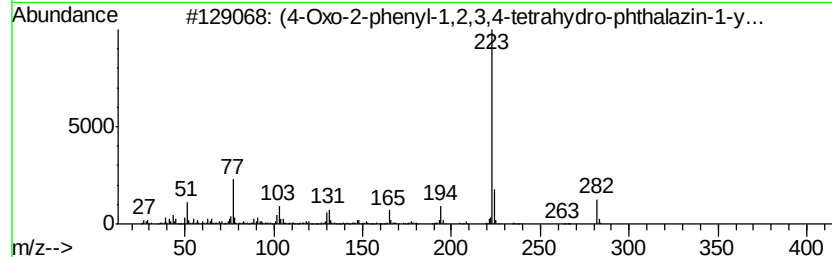
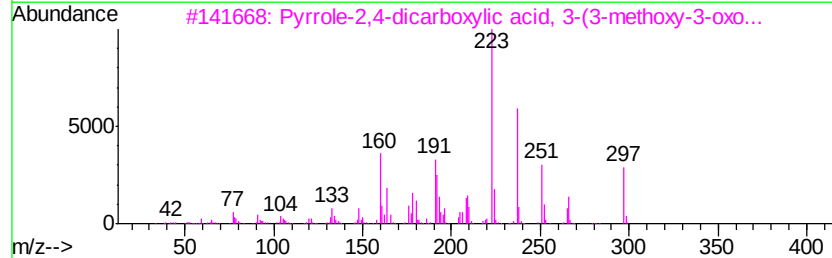
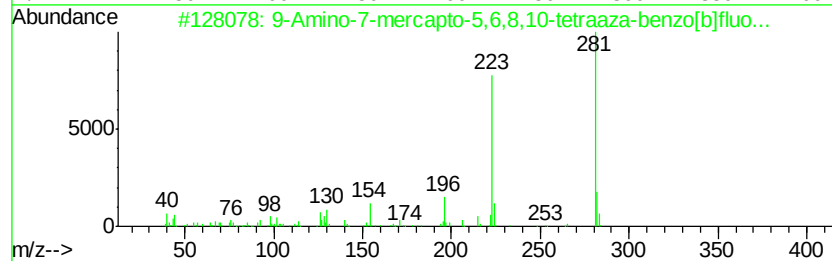
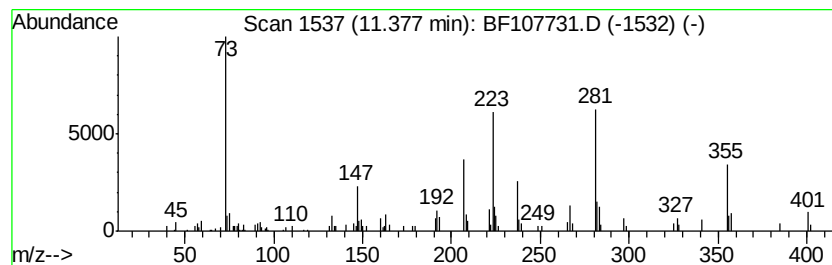
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 unknown11.38 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.38	2.05 ng	144831	Phenanthrene-d10	11.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Amino-7-mercapto-5,6,8,10-tetr...	281	C13H7N5OS	1000274-60-9	38
2		Pyrrole-2,4-dicarboxylic acid, 3...	297	C14H19N06	298686-26-7	30
3		(4-Oxo-2-phenyl-1,2,3,4-tetrahyd...	282	C16H14N2O3	1000190-14-1	18
4		Ketoprofen di-methyl derivative	282	C18H18O3	1000137-08-9	18
5		Benzenamine, N-[4-(1-methylethyl...	356	C20H24N2O2S	314765-47-4	18



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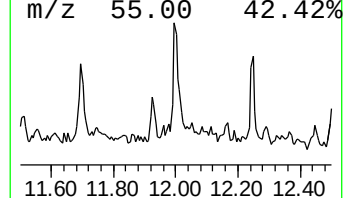
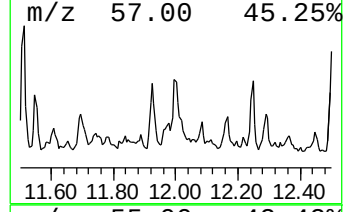
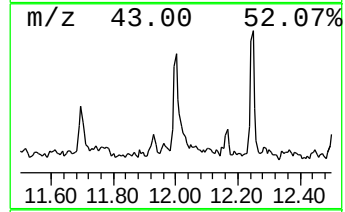
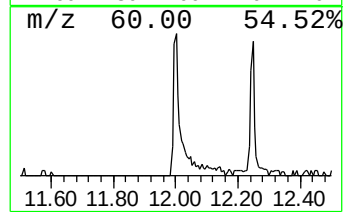
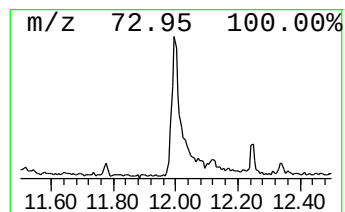
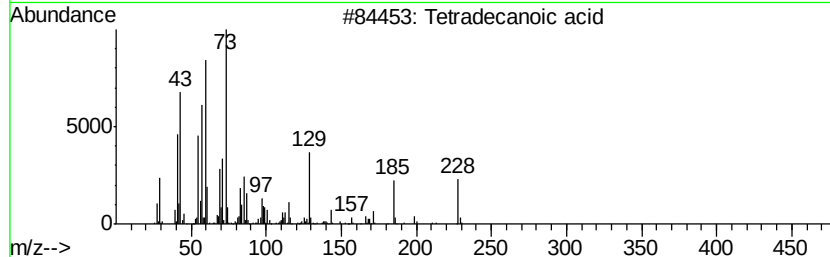
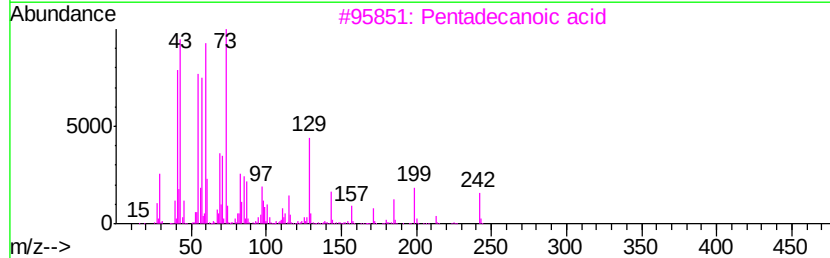
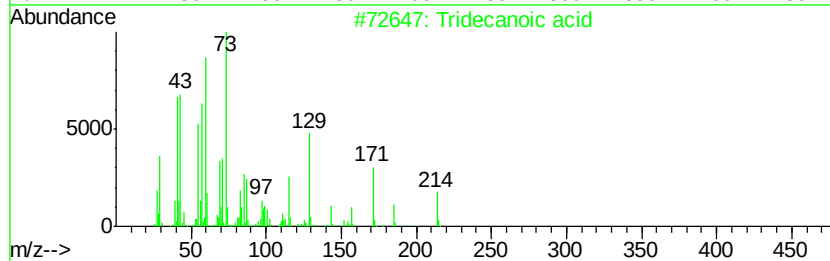
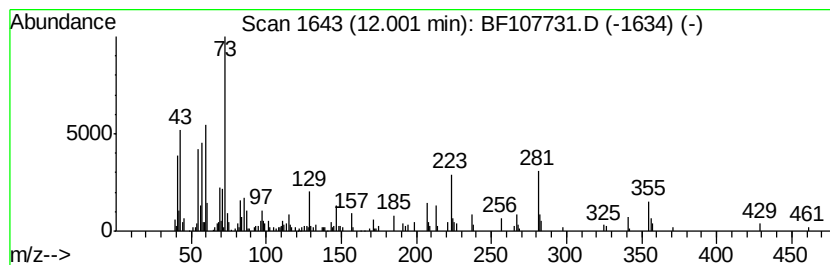
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 unknown12.00 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.00	5.36 ng	378504	Phenanthrene-d10	11.50

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecanoic acid	214	C13H26O2	000638-53-9	42
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	30
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	30
4		D-Ribose	150	C5H10O5	000050-69-1	27
5		Xylose	150	C5H10O5	000058-86-6	27



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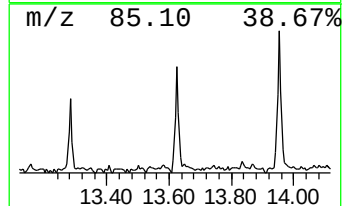
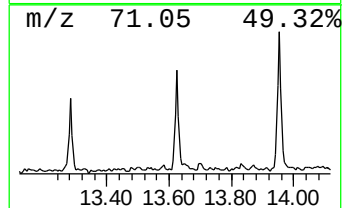
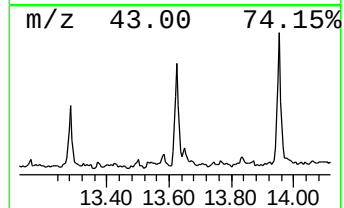
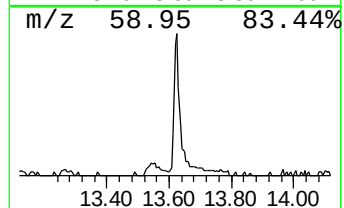
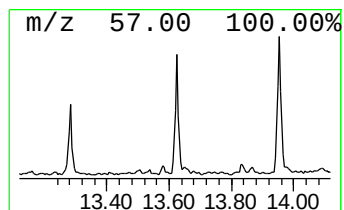
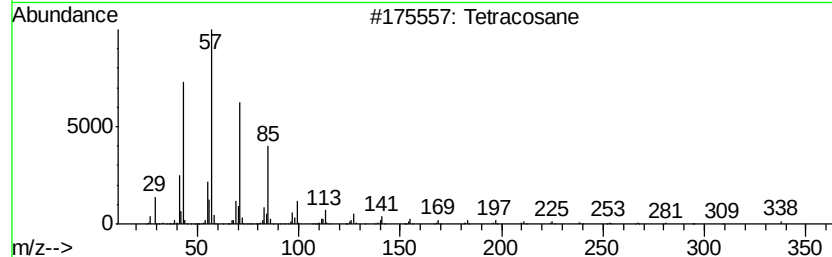
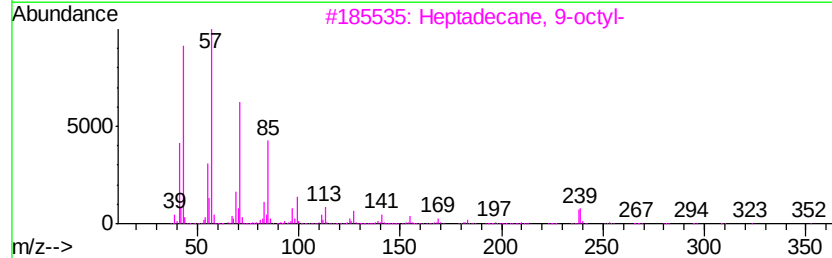
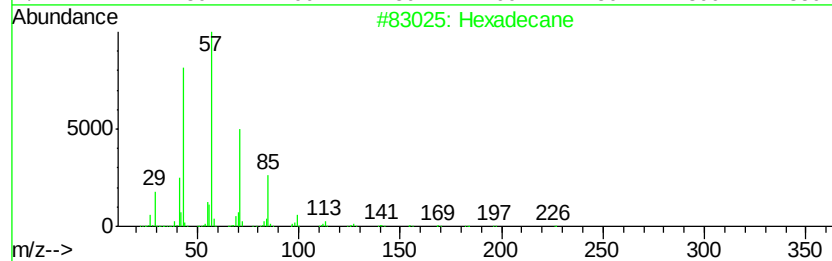
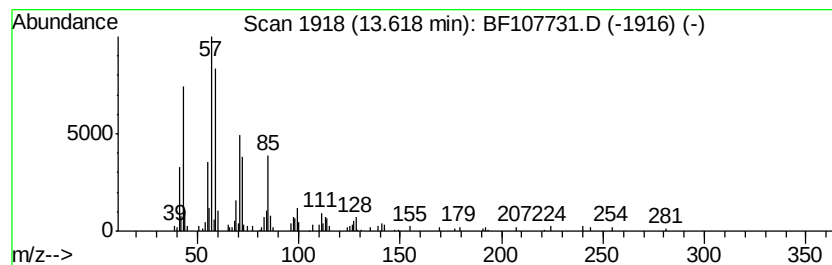
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Peak Number 6 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.62	2.49 ng	142735	Chrysene-d12		14.14
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	78
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	53
3	Tetracosane	338	C24H50	000646-31-1	53
4	Heneicosane	296	C21H44	000629-94-7	49
5	Heptadecane	240	C17H36	000629-78-7	46



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Sample : J4142-05
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

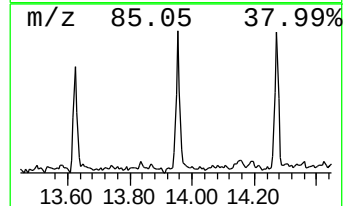
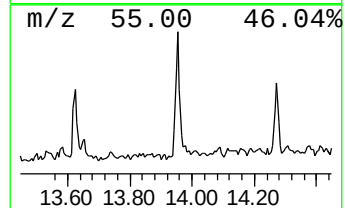
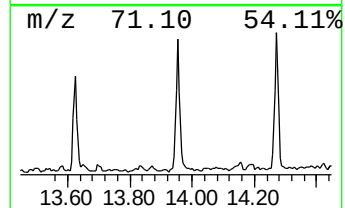
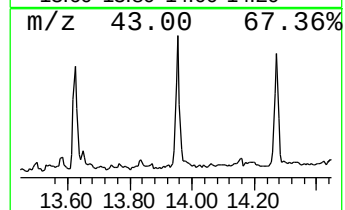
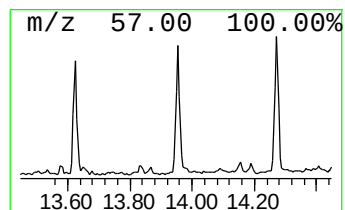
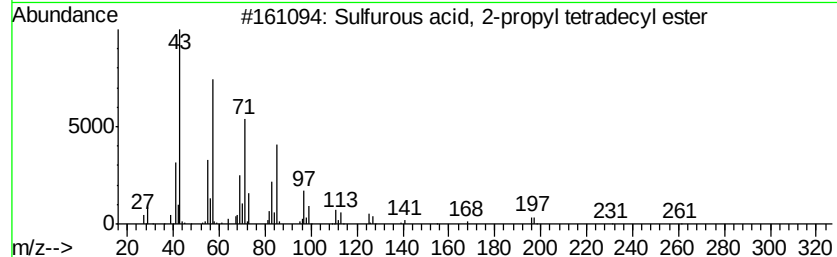
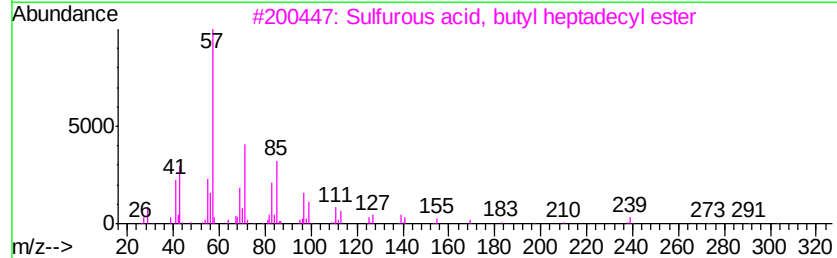
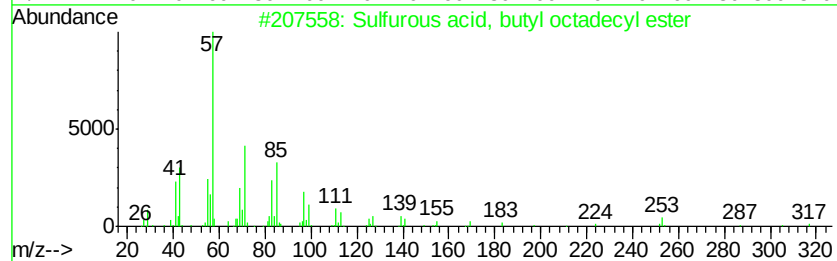
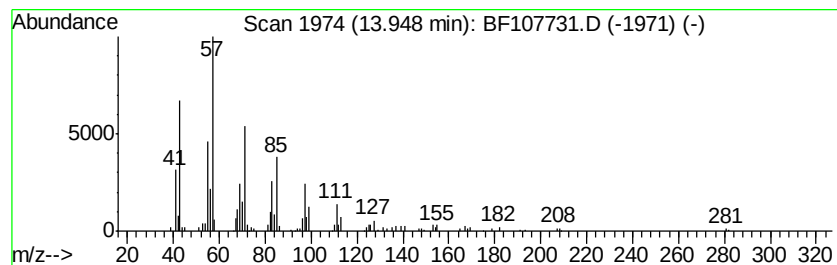
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Sulfurous acid, butyl octadecyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	3.57 ng	204628	Chrysene-d12	14.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	91
2		Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	90
3		Sulfurous acid, 2-propyl tetradec...	320	C17H36O3S	1000309-12-5	87
4		1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	87
5		Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
Data File : BF107731.D
Acq On : 27 Jul 2018 6:51
Operator : JU/SJ
Sample : J4142-05
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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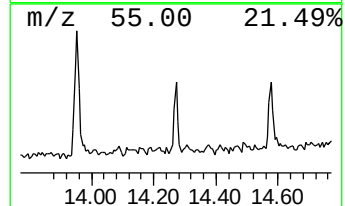
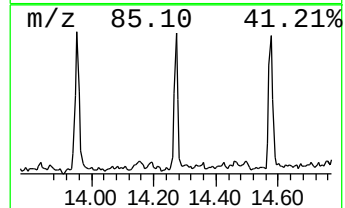
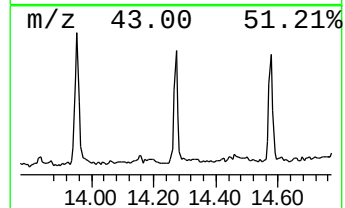
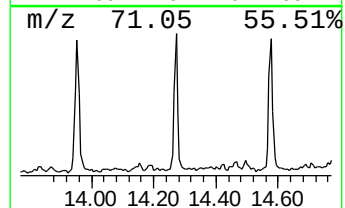
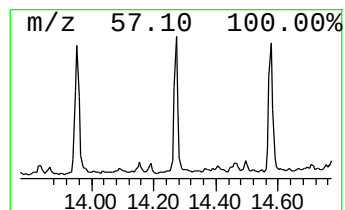
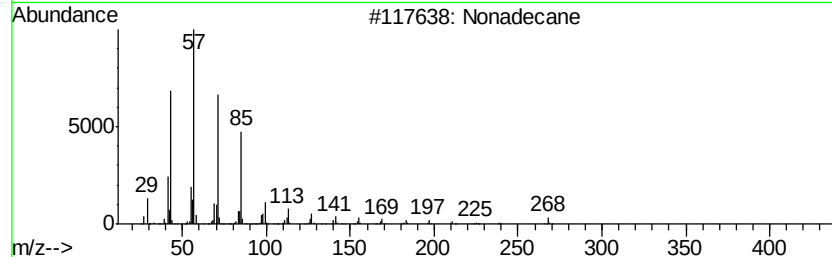
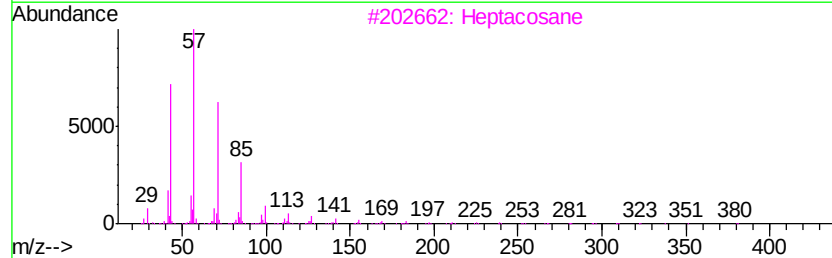
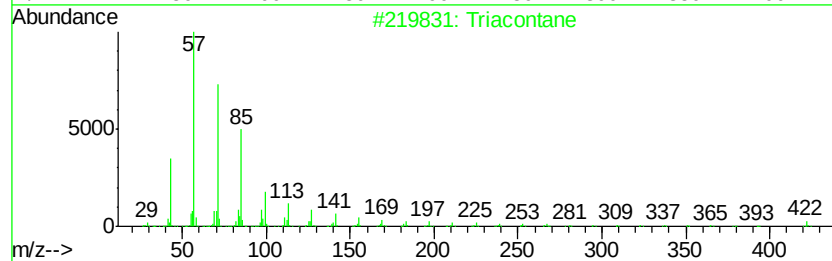
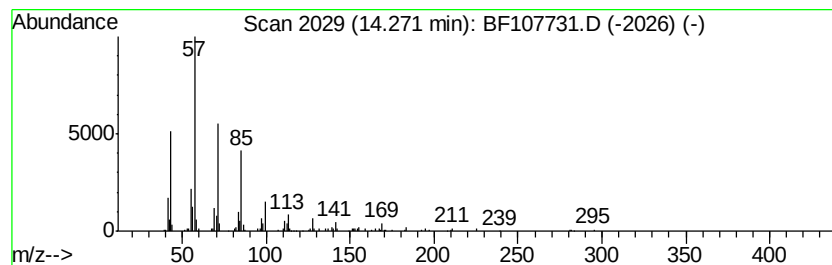
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Triacontane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.27	2.07 ng	118573	Chrysene-d12	14.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Triacontane	422	C30H62	000638-68-6	91
2		Heptacosane	380	C27H56	000593-49-7	91
3		Nonadecane	268	C19H40	000629-92-5	91
4		Heneicosane	296	C21H44	000629-94-7	87
5		Tetracosane	338	C24H50	000646-31-1	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
Data File : BF107731.D
Acq On : 27 Jul 2018 6:51
Operator : JU/SJ
Sample : J4142-05
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-1

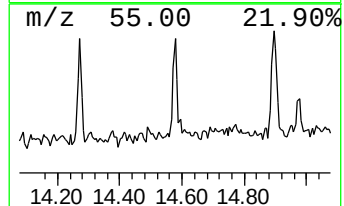
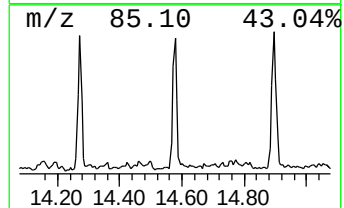
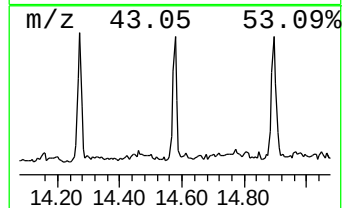
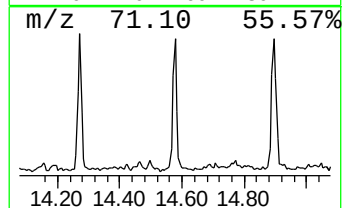
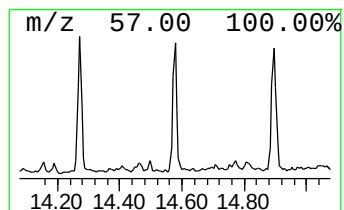
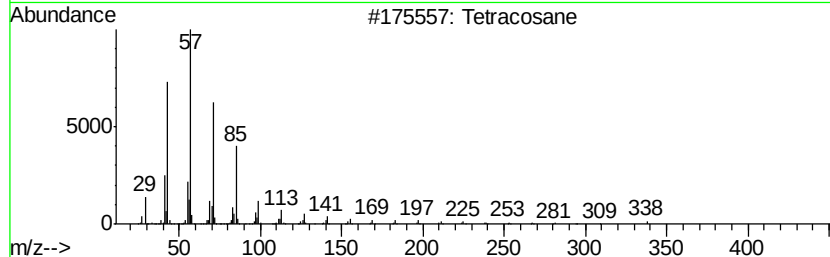
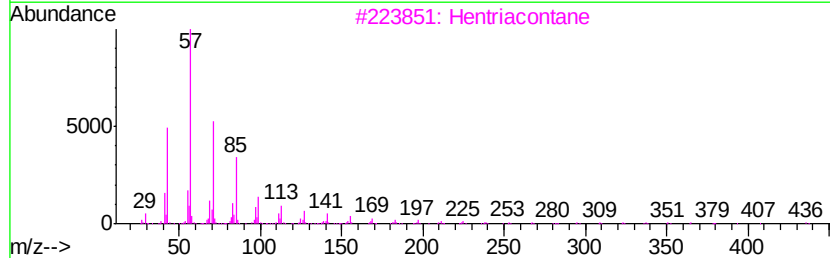
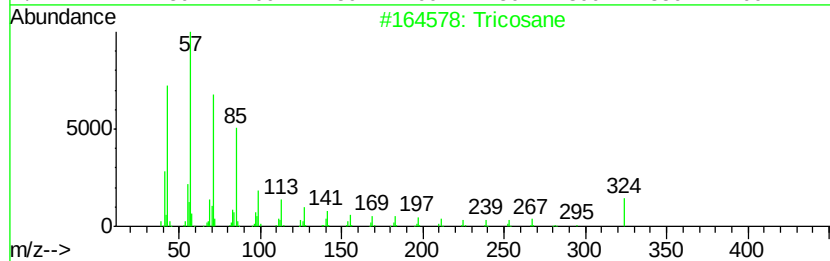
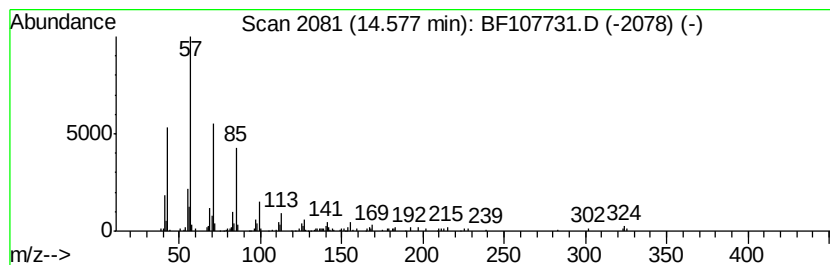
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hentriacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.58	2.50 ng	143647	Chrysene-d12	14.14

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane		324	C23H48	000638-67-5	94
2	Hentriacontane		437	C31H64	000630-04-6	90
3	Tetracosane		338	C24H50	000646-31-1	90
4	Docosane		310	C22H46	000629-97-0	87
5	Eicosane		282	C20H42	000112-95-8	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
Data File : BF107731.D
Acq On : 27 Jul 2018 6:51
Operator : JU/SJ
Sample : J4142-05
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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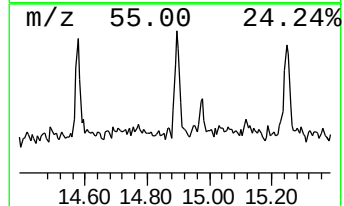
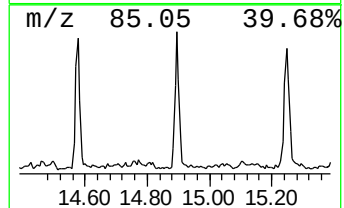
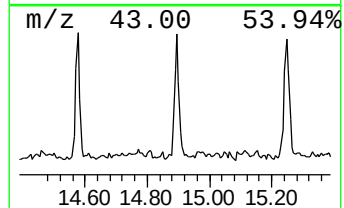
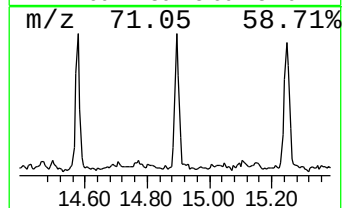
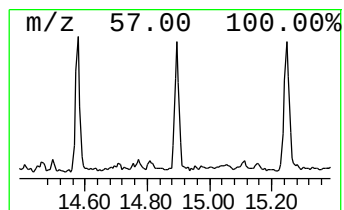
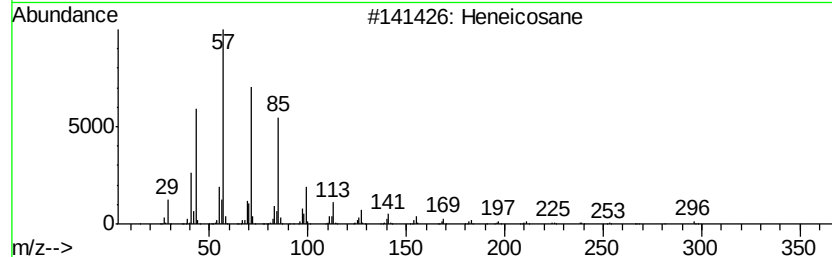
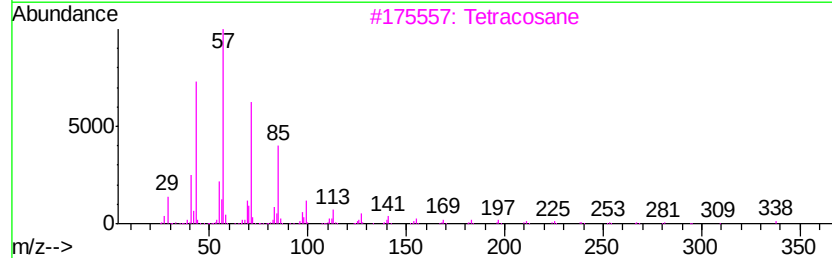
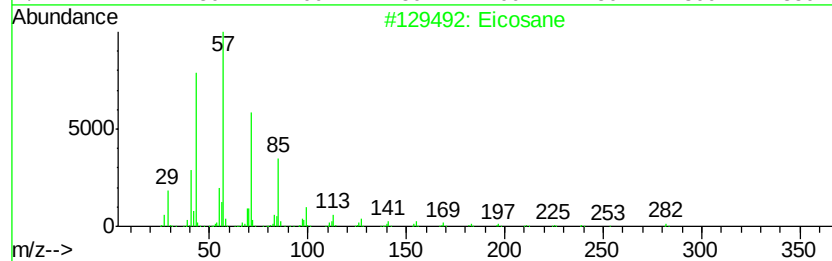
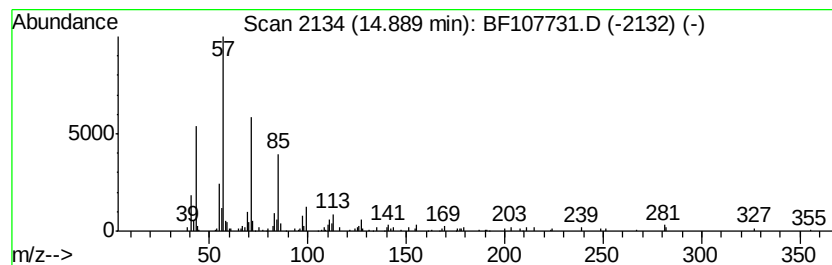
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.89	2.70 ng	154823	Chrysene-d12	14.14

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	94
2	Tetracosane		338	C24H50	000646-31-1	91
3	Heneicosane		296	C21H44	000629-94-7	90
4	Hentriacontane		437	C31H64	000630-04-6	90
5	Hexacosane		366	C26H54	000630-01-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
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Acq On : 27 Jul 2018 6:51
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Sample : J4142-05
Misc :
ALS Vial : 33 Sample Multiplier: 1

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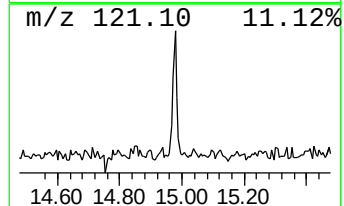
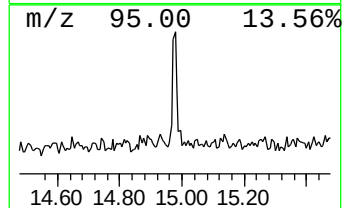
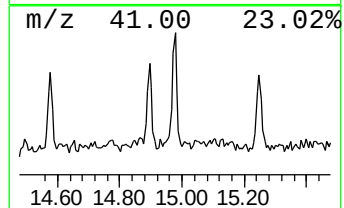
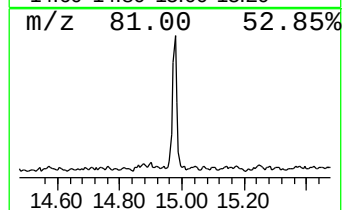
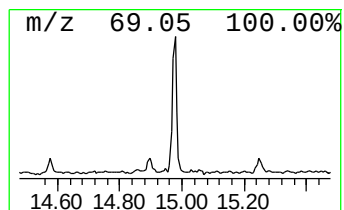
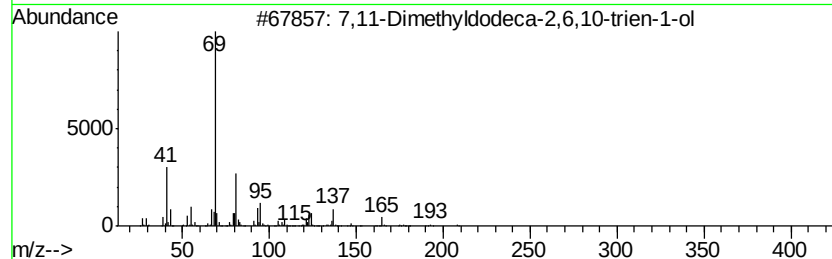
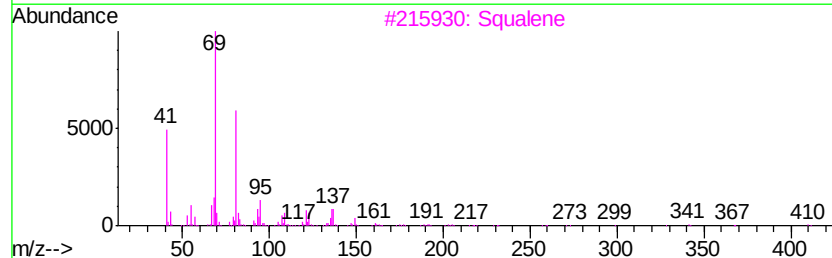
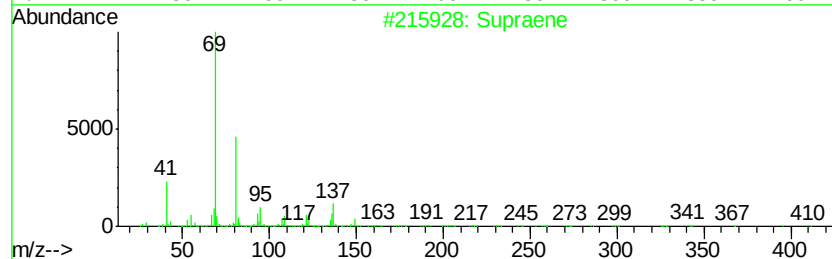
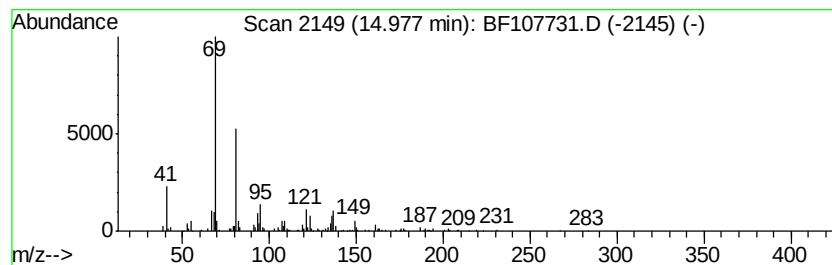
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Supraene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	2.16 ng	133753	Perylene-d12	15.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	91
2		Squalene	410	C30H50	000111-02-4	91
3		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
4		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
5		2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
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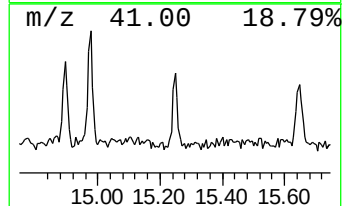
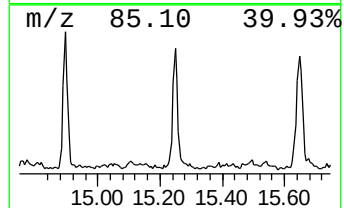
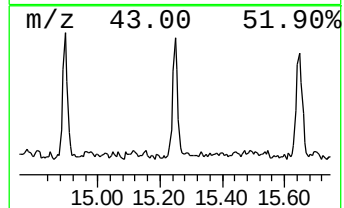
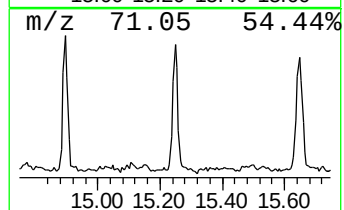
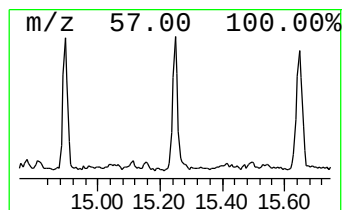
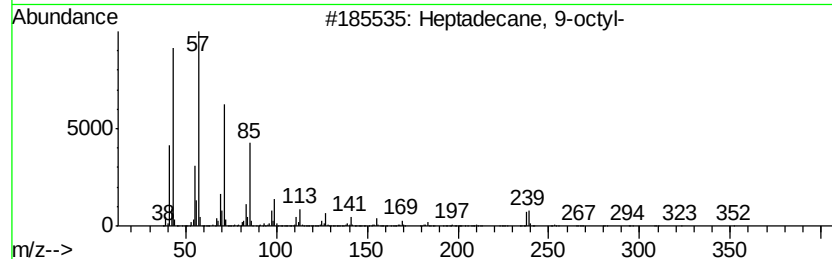
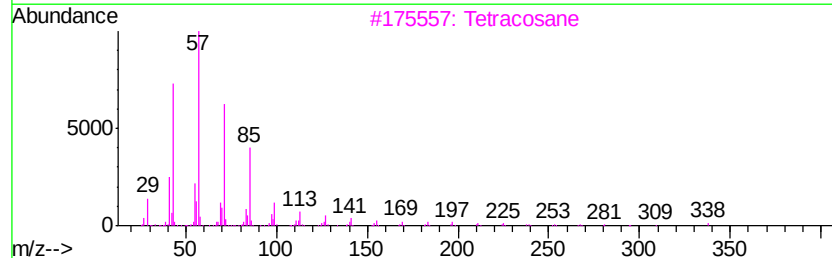
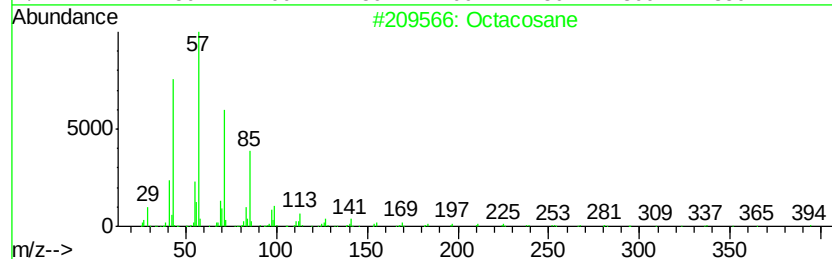
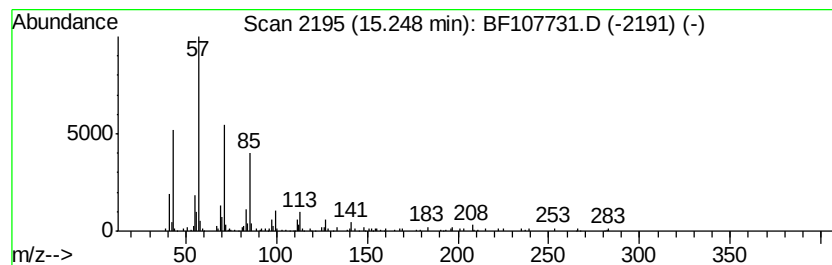
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.25	2.52 ng	156208	Perylene-d12	15.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	90
2		Tetracosane	338	C24H50	000646-31-1	90
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
4		2-Bromo dodecane	248	C12H25Br	013187-99-0	86
5		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
Data File : BF107731.D
Acq On : 27 Jul 2018 6:51
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Sample : J4142-05
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ClientSampleId :
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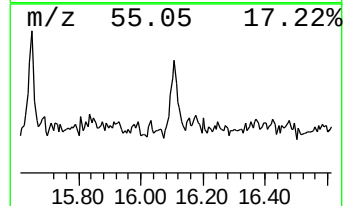
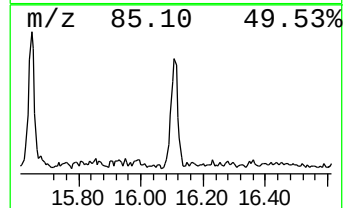
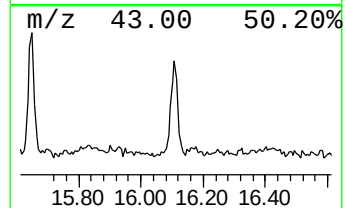
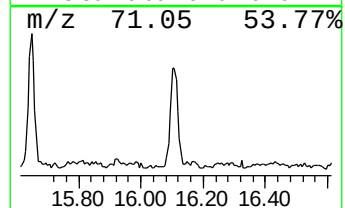
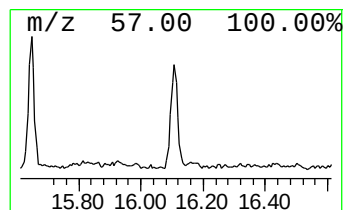
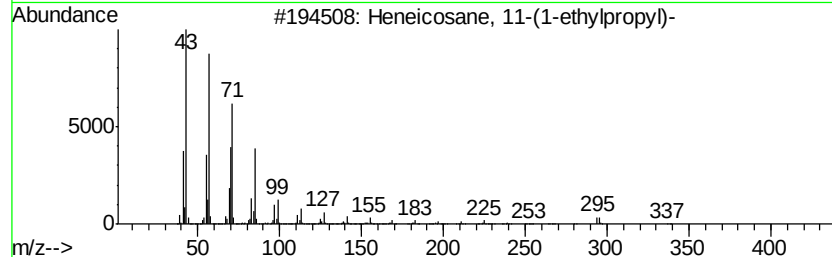
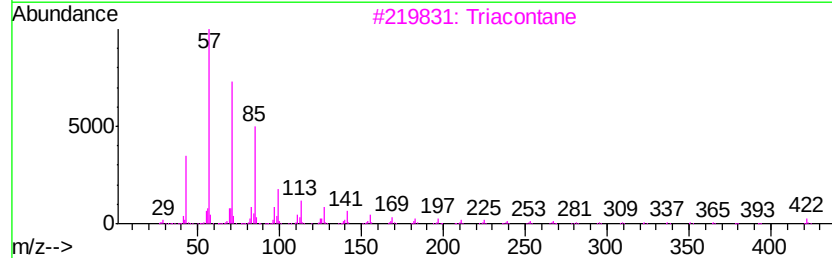
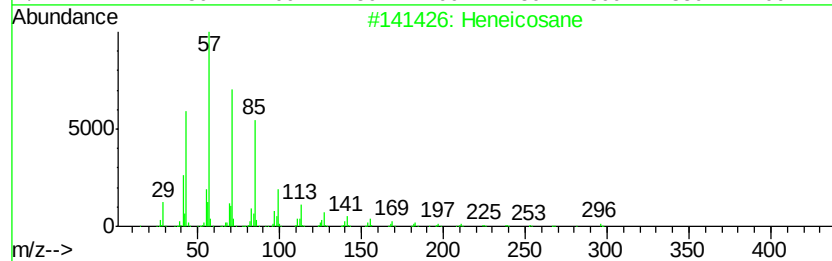
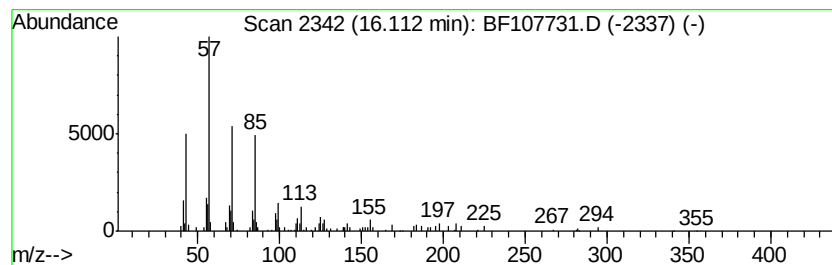
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.11	2.35 ng	146036	Perylene-d12	15.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	90
2		Triacontane	422	C30H62	000638-68-6	87
3		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86
4		Tetracosane	338	C24H50	000646-31-1	83
5		Heptadecane	240	C17H36	000629-78-7	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
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Acq On : 27 Jul 2018 6:51
Operator : JU/SJ
Sample : J4142-05
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

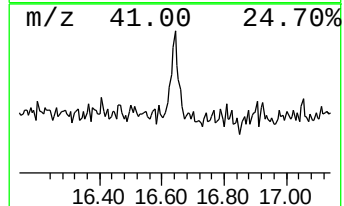
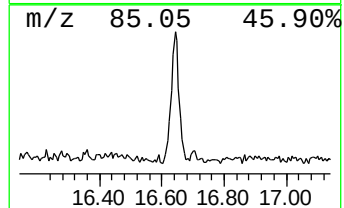
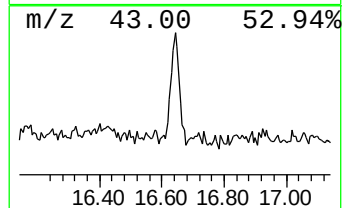
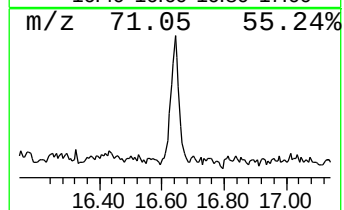
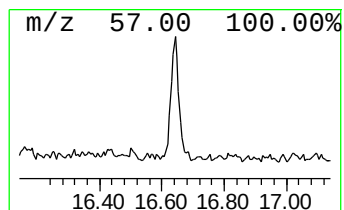
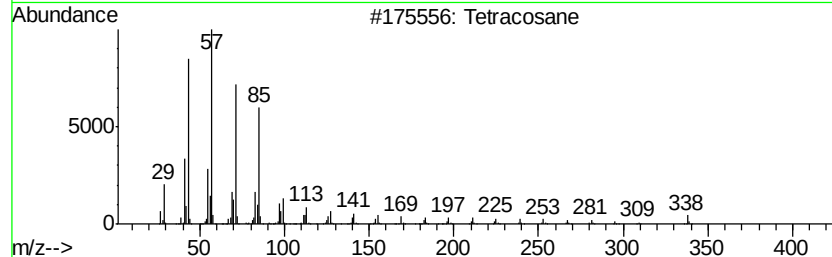
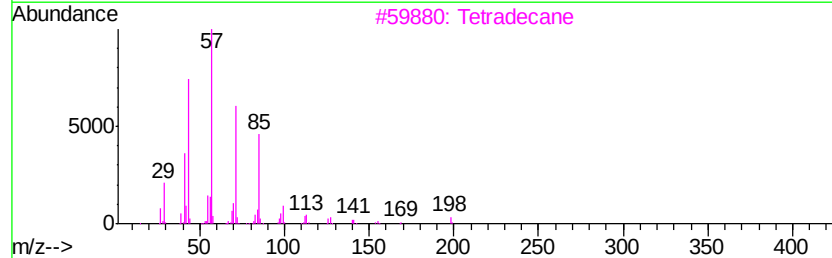
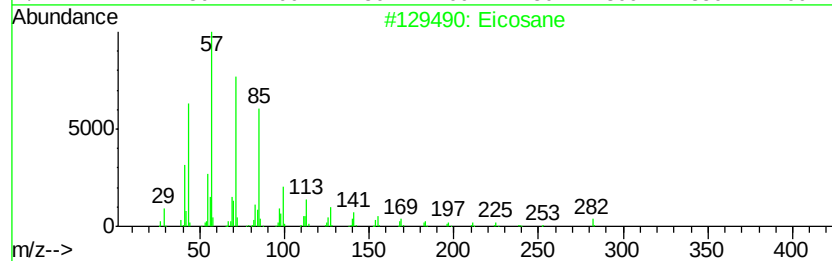
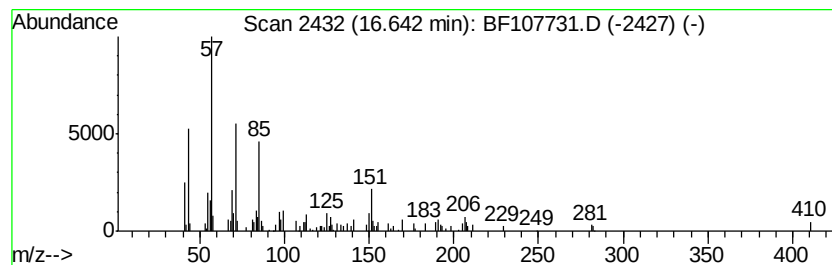
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Eicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.64	2.29 ng	142006	Perylene-d12	15.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	92
2		Tetradecane	198	C14H30	000629-59-4	64
3		Tetracosane	338	C24H50	000646-31-1	62
4		Octacosane	394	C28H58	000630-02-4	62
5		Hexacosane	366	C26H54	000630-01-3	62



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
 Data File : BF107731.D
 Acq On : 27 Jul 2018 6:51
 Operator : JU/SJ
 Sample : J4142-05
 Misc :
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.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...	5.19	3.3	ng	175447	1	6.97	1054090	20.0
unknown6.73	6.73	78.4	ng	4133360	1	6.97	1054090	20.0
unknown11.38	11.38	2.0	ng	144831	4	11.50	1411320	20.0
unknown12.00	12.00	5.4	ng	378504	4	11.50	1411320	20.0
Hexadecane	13.62	2.5	ng	142735	5	14.14	1147900	20.0
Sulfurous acid, b...	13.95	3.6	ng	204628	5	14.14	1147900	20.0
triacontane	14.27	2.1	ng	118573	5	14.14	1147900	20.0
Hentriacontane	14.58	2.5	ng	143647	5	14.14	1147900	20.0
Eicosane	14.89	2.7	ng	154823	5	14.14	1147900	20.0
Supraene	14.98	2.2	ng	133753	6	15.67	1240960	20.0
Octacosane	15.25	2.5	ng	156208	6	15.67	1240960	20.0
Heneicosane	16.11	2.4	ng	146036	6	15.67	1240960	20.0
Eicosane	16.64	2.3	ng	142006	6	15.67	1240960	20.0