

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072718\
 Data File : BF107753.D
 Acq On : 27 Jul 2018 18:34
 Operator : JU/SJ
 Sample : J4189-15
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-14-S

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-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	5.196	482	486	502	rBV	347923	483399	14.25%	1.656%
2	5.596	550	554	581	rBV	1519272	2547362	75.11%	8.729%
3	6.596	721	724	744	rBV	1604594	2742853	80.88%	9.399%
4	6.731	744	747	783	rVV	2218187	3391359	100.00%	11.621%
5	6.960	783	786	808	rVV	504088	979087	28.87%	3.355%
6	7.113	809	812	837	rVB	2017114	2413051	71.15%	8.269%
7	7.525	879	882	906	rBV	1061067	1863395	54.95%	6.385%
8	8.242	1000	1004	1023	rBV	868402	1188082	35.03%	4.071%
9	9.313	1182	1186	1213	rBV	2958099	3383669	99.77%	11.595%
10	9.707	1249	1253	1264	rBV	193392	210553	6.21%	0.721%
11	10.001	1299	1303	1325	rBV	1068149	1251510	36.90%	4.288%
12	10.795	1434	1438	1451	rBV	1278781	1764527	52.03%	6.046%
13	11.495	1553	1557	1569	rBV	855468	1126110	33.21%	3.859%
14	11.995	1639	1642	1646	rBV2	36610	46453	1.37%	0.159%
15	12.713	1760	1764	1772	rBV	56611	70418	2.08%	0.241%
16	12.942	1798	1803	1808	rBV	60441	94885	2.80%	0.325%
17	13.077	1822	1826	1838	rBV	2403686	2547551	75.12%	8.730%
18	13.954	1972	1975	1982	rBV	133286	151359	4.46%	0.519%
19	14.142	2003	2007	2020	rBV	890813	1243006	36.65%	4.259%
20	14.577	2078	2081	2090	rBV	60307	82838	2.44%	0.284%
21	14.895	2132	2135	2141	rBV	60681	70555	2.08%	0.242%
22	14.977	2145	2149	2153	rVB	116754	115861	3.42%	0.397%
23	15.248	2192	2195	2199	rVB2	76750	85083	2.51%	0.292%
24	15.677	2260	2268	2279	rBV	600641	1094851	32.28%	3.752%
25	16.107	2337	2341	2347	rVB	81887	117397	3.46%	0.402%
26	16.642	2428	2432	2440	rVB4	62218	117986	3.48%	0.404%

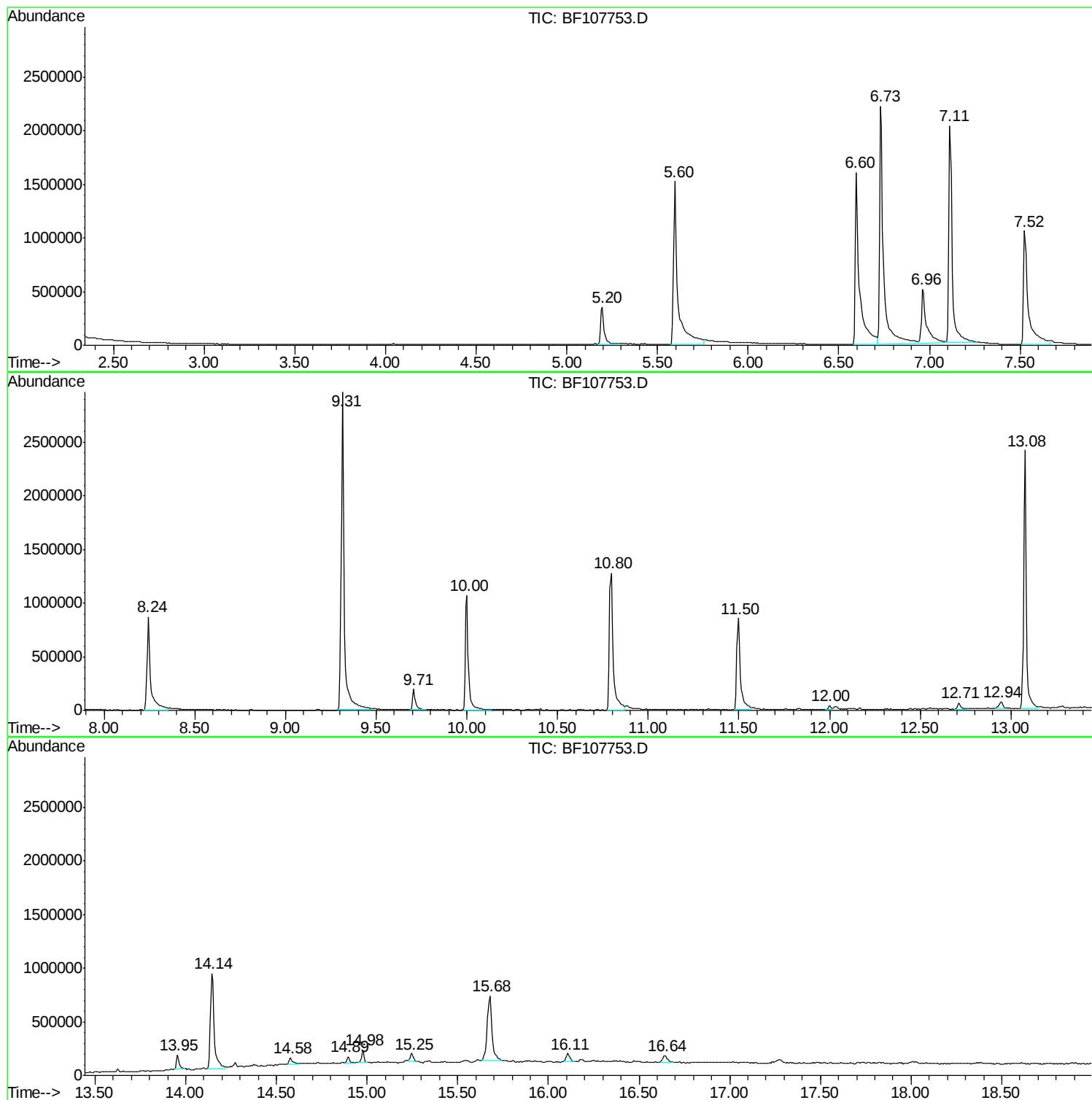
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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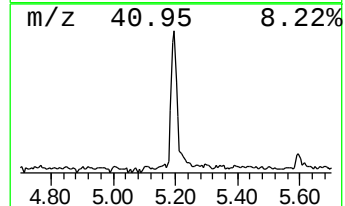
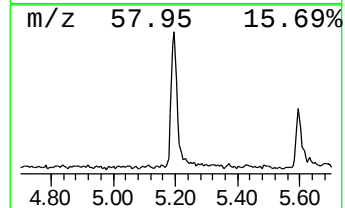
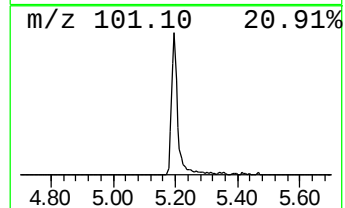
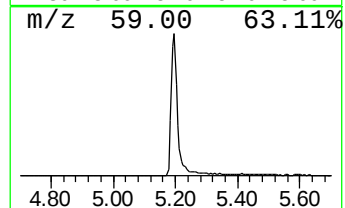
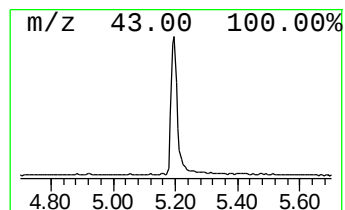
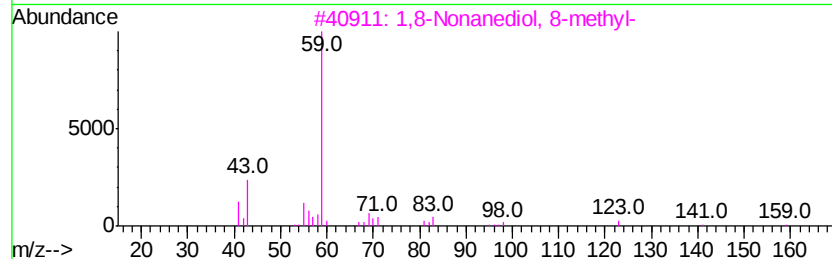
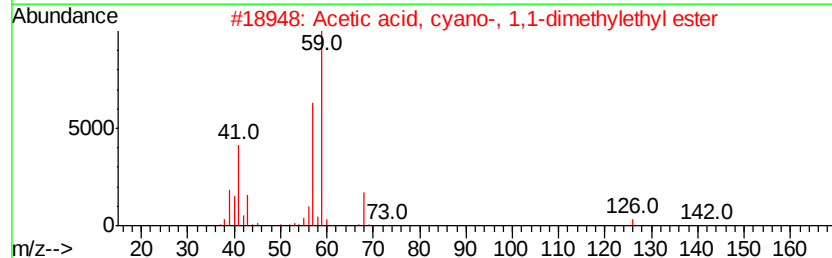
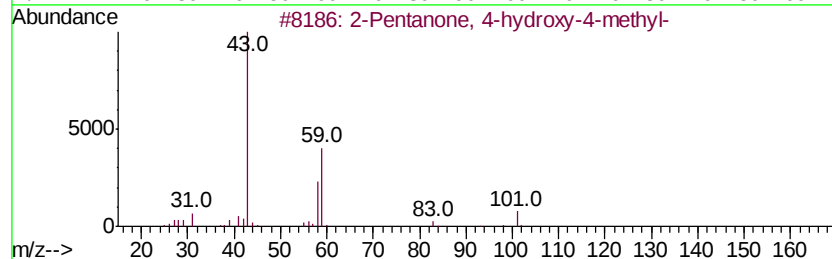
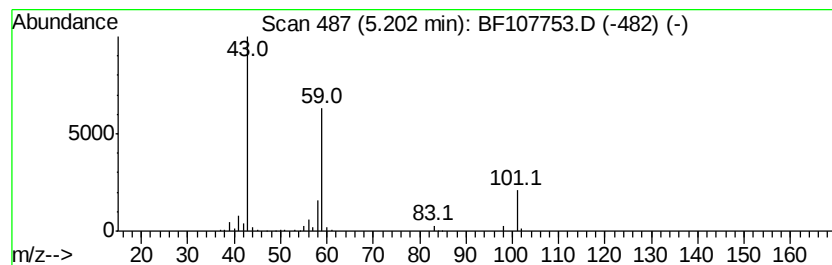
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	9.87 ng	483399	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	56
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
4			Acetone	58	C3H6O	000067-64-1	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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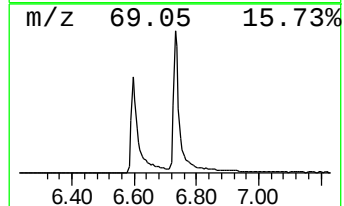
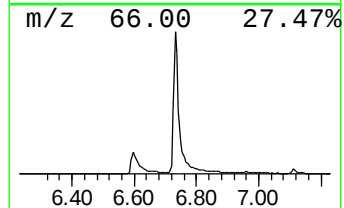
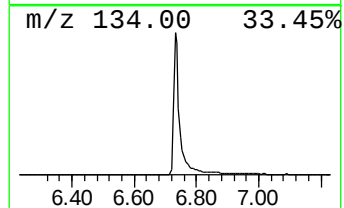
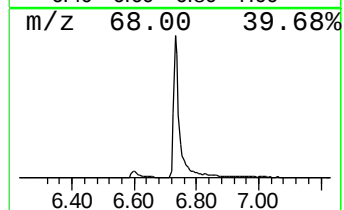
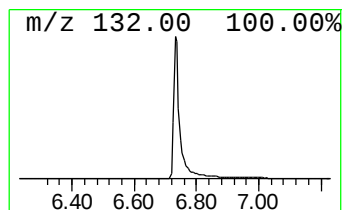
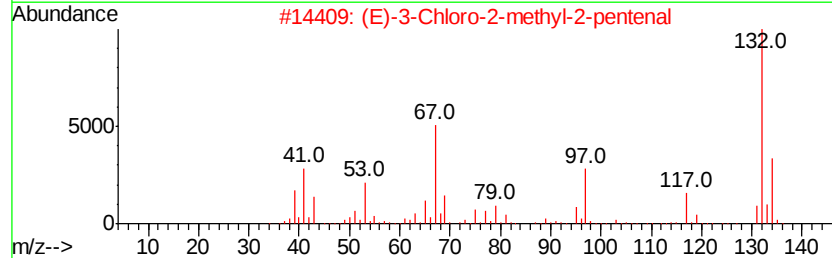
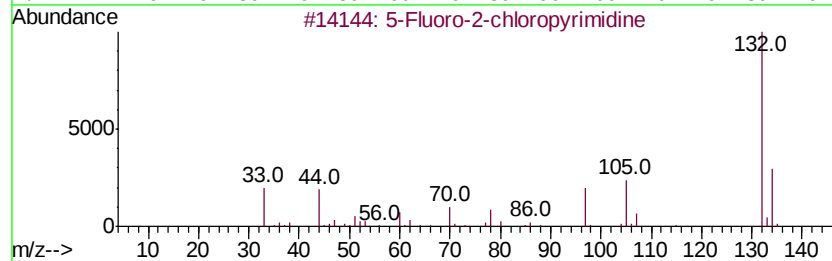
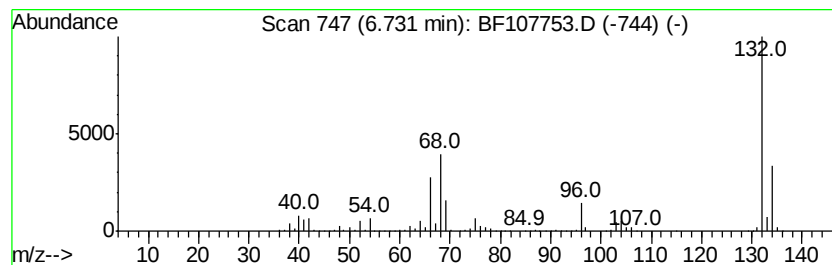
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Peak Number 2 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	69.28 ng	3391360	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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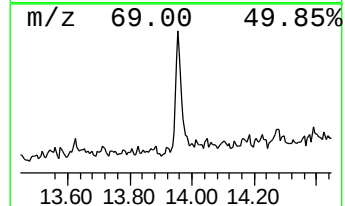
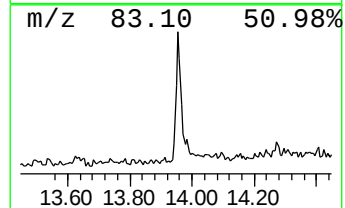
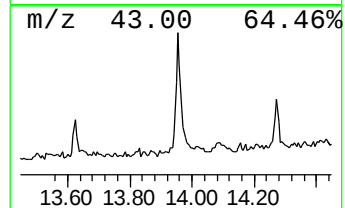
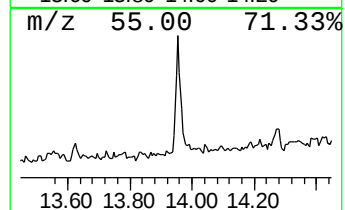
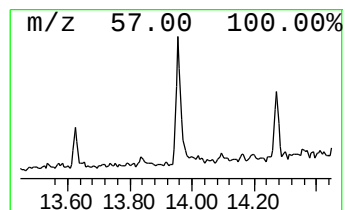
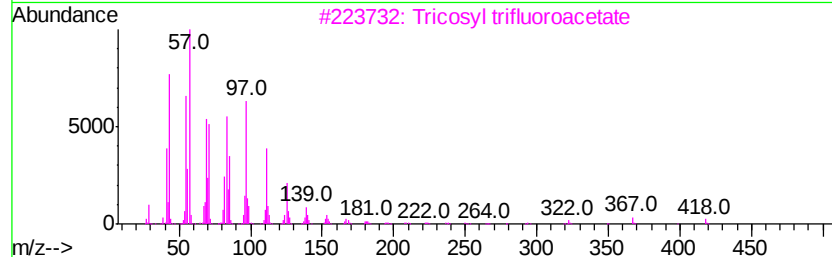
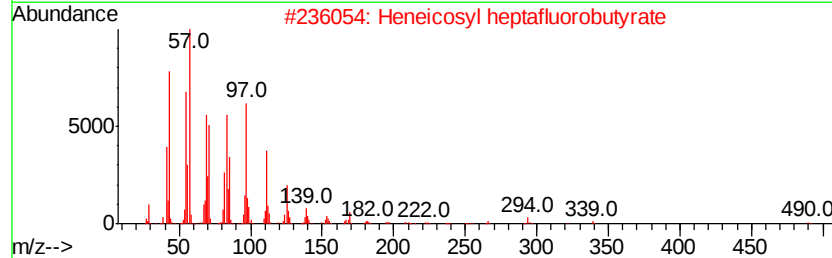
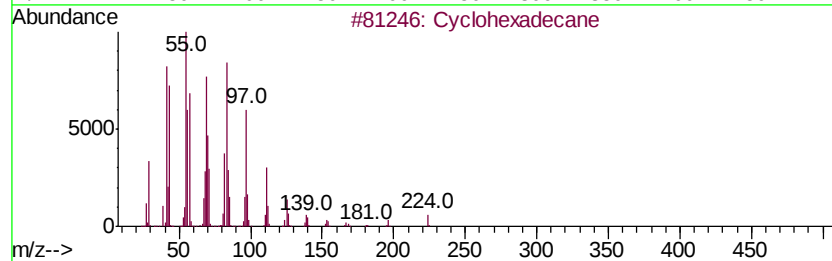
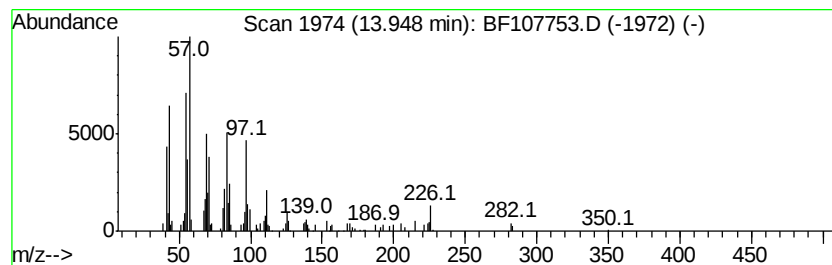
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Peak Number 4 Cyclohexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	2.44 ng	151359	Chrysene-d12	14.14

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexadecane	224	C16H32	000295-65-8	95
2		Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91
3		Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
4		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
5		Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	91



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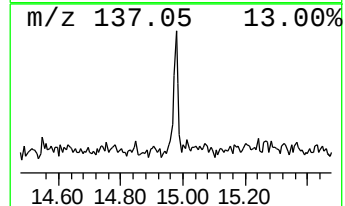
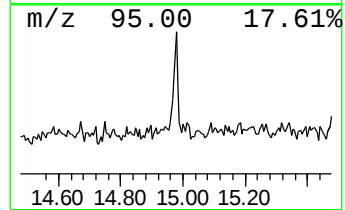
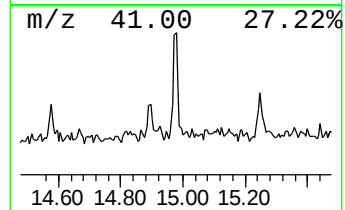
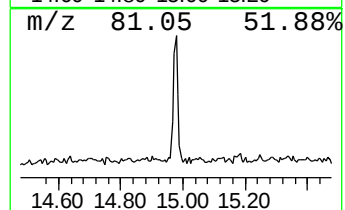
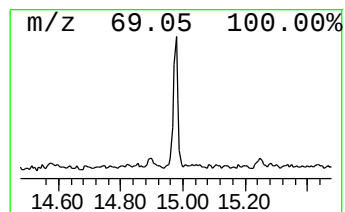
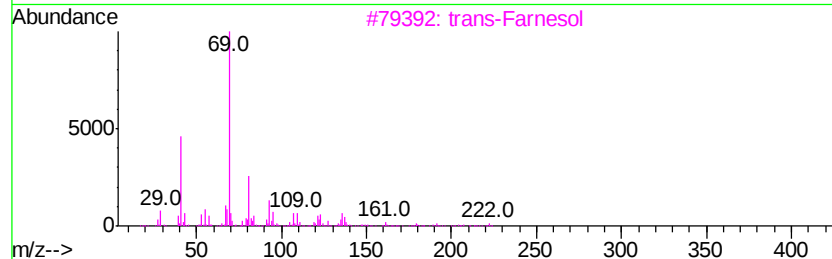
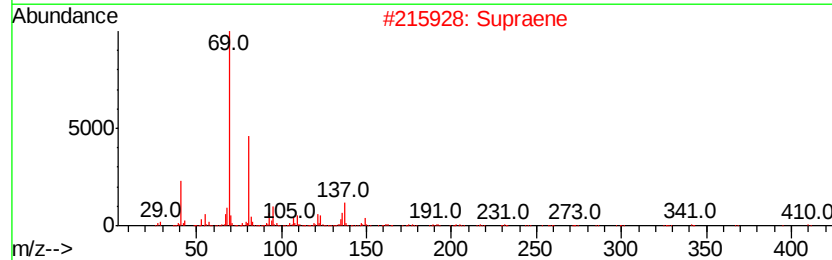
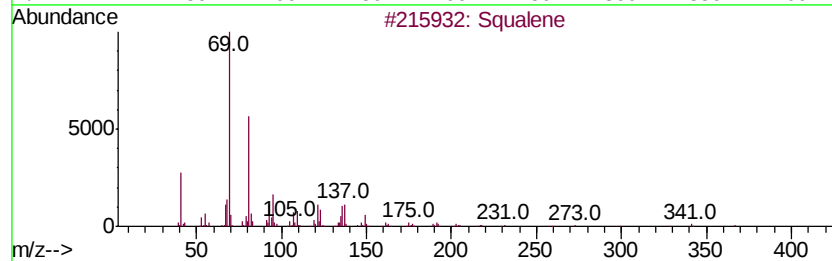
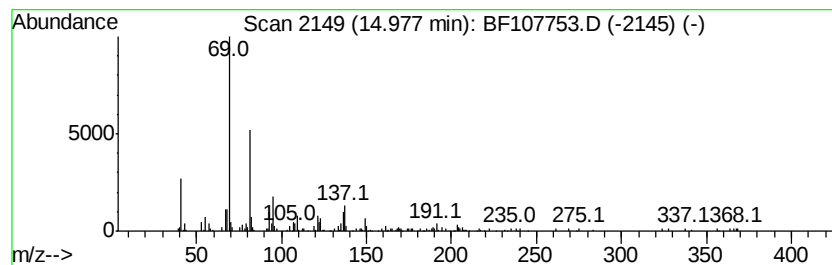
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Peak Number 5 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	2.12 ng	115861	Perylene-d12	15.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	87
2		Supraene	410	C30H50	007683-64-9	83
3		trans-Farnesol	222	C15H26O	000106-28-5	81
4		Farnesol isomer a	222	C15H26O	1000108-92-4	74
5		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64



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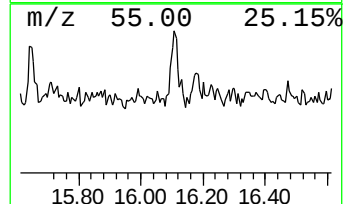
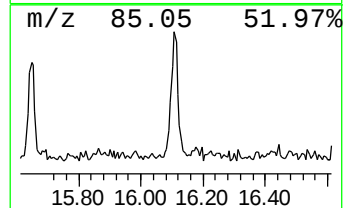
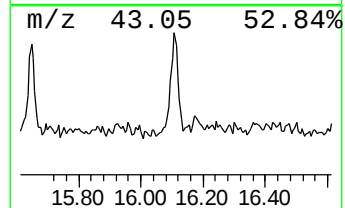
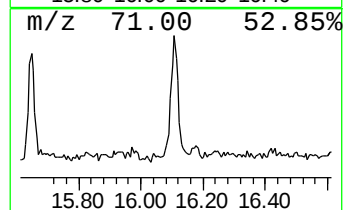
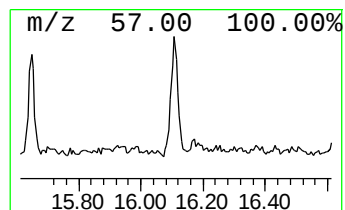
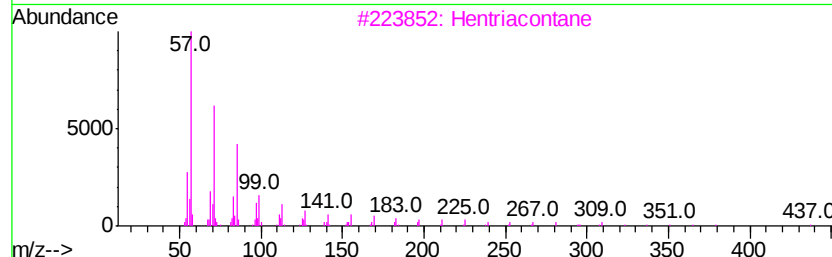
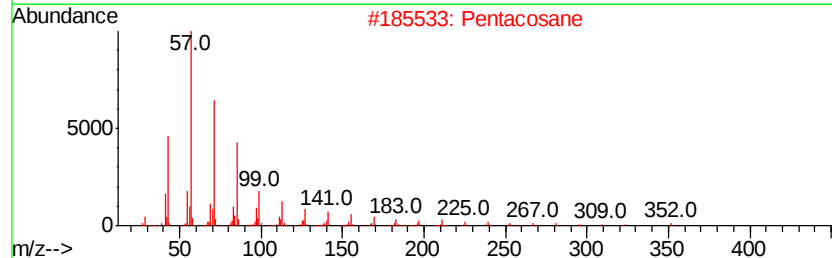
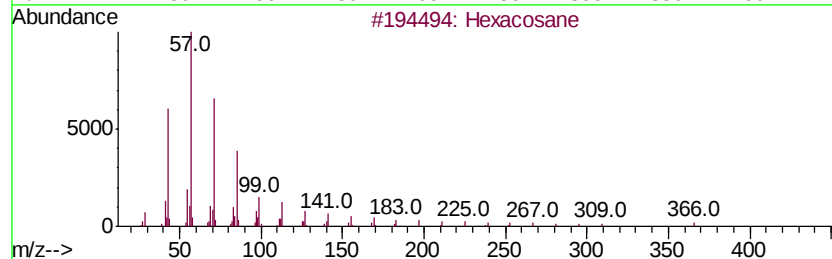
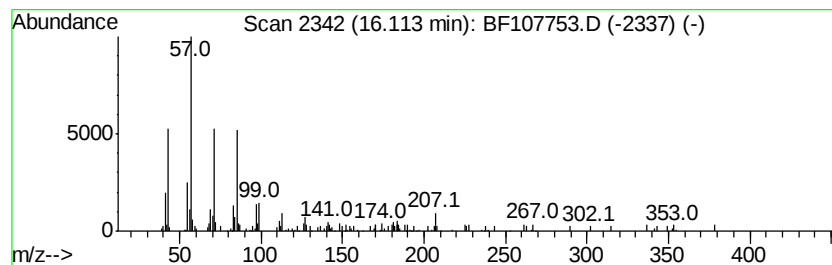
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.11	2.14 ng	117397	Perylene-d12	15.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	96
2		Pentacosane	352	C25H52	000629-99-2	95
3		Hentriacontane	437	C31H64	000630-04-6	87
4		Tetracosane	338	C24H50	000646-31-1	87
5		Tetratetracontane	619	C44H90	007098-22-8	87



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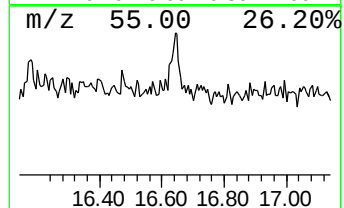
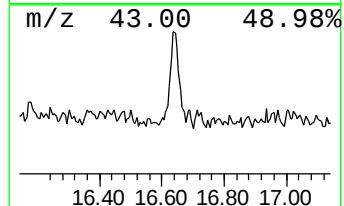
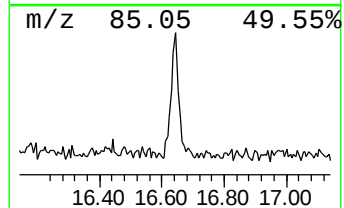
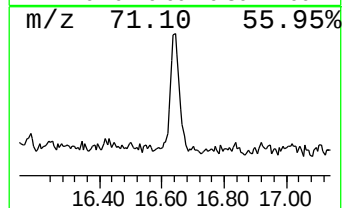
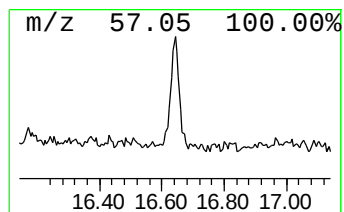
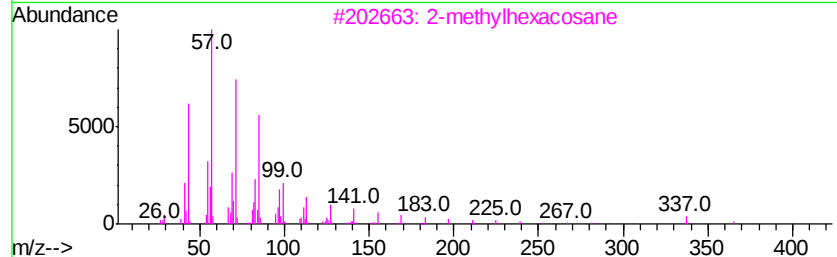
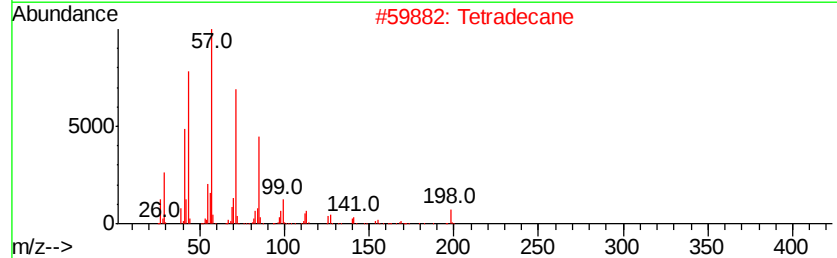
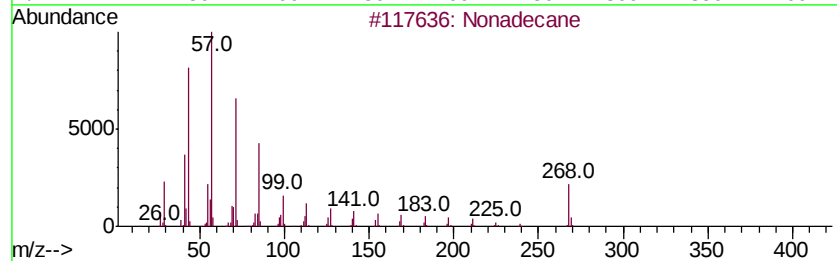
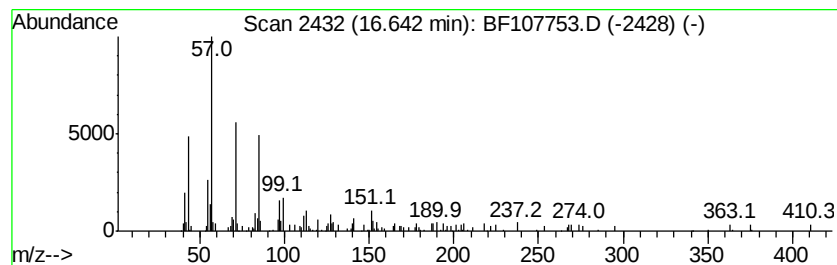
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Nonadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.64	2.16 ng	117986	Perylene-d12	15.68

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane		268	C19H40	000629-92-5	64
2	Tetradecane		198	C14H30	000629-59-4	58
3	2-methylhexacosane		380	C27H56	1000376-72-7	58
4	Octacosane		394	C28H58	000630-02-4	52
5	Heneicosane		296	C21H44	000629-94-7	52



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072718\
Data File : BF107753.D
Acq On : 27 Jul 2018 18:34
Operator : JU/SJ
Sample : J4189-15
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-14-S

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...	5.20	9.9	ng	483399	1	6.97	979087	20.0
unknown6.73	6.73	69.3	ng	3391360	1	6.97	979087	20.0
Cyclohexadecane	13.95	2.4	ng	151359	5	14.14	1243010	20.0
Squalene	14.98	2.1	ng	115861	6	15.68	1094850	20.0
Hexacosane	16.11	2.1	ng	117397	6	15.68	1094850	20.0
Nonadecane	16.64	2.2	ng	117986	6	15.68	1094850	20.0