

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082718\
 Data File : BF108515.D
 Acq On : 27 Aug 2018 17:21
 Operator : JU/SJ
 Sample : J4538-02
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VSS2

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-BF080818.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	5.243	490	494	506	rVB	176436	207680	7.36%	0.867%
2	5.631	555	560	563	rBV	2408093	2206609	78.20%	9.214%
3	6.625	724	729	732	rBV	2372959	2378539	84.29%	9.932%
4	6.772	749	754	757	rBV	2711791	2407282	85.31%	10.052%
5	7.001	789	793	796	rBV	807161	720051	25.52%	3.007%
6	7.154	815	819	823	rBV	2223242	1940715	68.77%	8.104%
7	7.560	883	888	891	rBV	1716973	1564585	55.44%	6.533%
8	8.284	1007	1011	1014	rBV	1045795	890092	31.54%	3.717%
9	9.354	1189	1193	1202	rBV	3144638	2821906	100.00%	11.784%
10	9.530	1220	1223	1227	rVB	105660	88322	3.13%	0.369%
11	9.689	1247	1250	1254	rVB3	36197	30680	1.09%	0.128%
12	9.742	1256	1259	1265	rBV	204324	179213	6.35%	0.748%
13	10.042	1301	1310	1321	rBV2	1134485	1039069	36.82%	4.339%
14	10.836	1441	1445	1458	rBV	1672893	1489779	52.79%	6.221%
15	11.536	1561	1564	1568	rBV	933857	881503	31.24%	3.681%
16	12.042	1647	1650	1654	rBV	40161	37153	1.32%	0.155%
17	13.124	1830	1834	1837	rBV	2174287	1879360	66.60%	7.848%
18	14.036	1985	1989	2001	rVB3	65154	145965	5.17%	0.610%
19	14.189	2011	2015	2019	rBV	795092	763698	27.06%	3.189%
20	14.318	2034	2037	2040	rBV	38311	32866	1.16%	0.137%
21	14.624	2086	2089	2094	rVB	62825	61668	2.19%	0.258%
22	14.824	2120	2123	2128	rVB	43783	49786	1.76%	0.208%
23	14.948	2141	2144	2148	rBV	58337	69483	2.46%	0.290%
24	15.036	2156	2159	2162	rBV	26694	31784	1.13%	0.133%
25	15.112	2168	2172	2180	rVB	122569	151617	5.37%	0.633%
26	15.312	2202	2206	2211	rVB	143599	168320	5.96%	0.703%
27	15.401	2215	2221	2231	rBV4	51792	154843	5.49%	0.647%
28	15.748	2272	2280	2285	rBV	514489	777184	27.54%	3.245%
29	15.948	2310	2314	2321	rVB2	58127	81503	2.89%	0.340%
30	16.195	2351	2356	2365	rVB	213696	337495	11.96%	1.409%
31	16.342	2375	2381	2383	rBV5	20393	43220	1.53%	0.180%
32	16.565	2417	2419	2427	rVB6	21697	35763	1.27%	0.149%
33	16.748	2444	2450	2455	rBV3	43241	89920	3.19%	0.375%
34	17.071	2501	2505	2515	rVB3	38665	76980	2.73%	0.321%

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ALS Vial : 19 Sample Multiplier: 1

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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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35	17.401	2555	2561	2568	rVB	51738	112667	3.99%	0.470%
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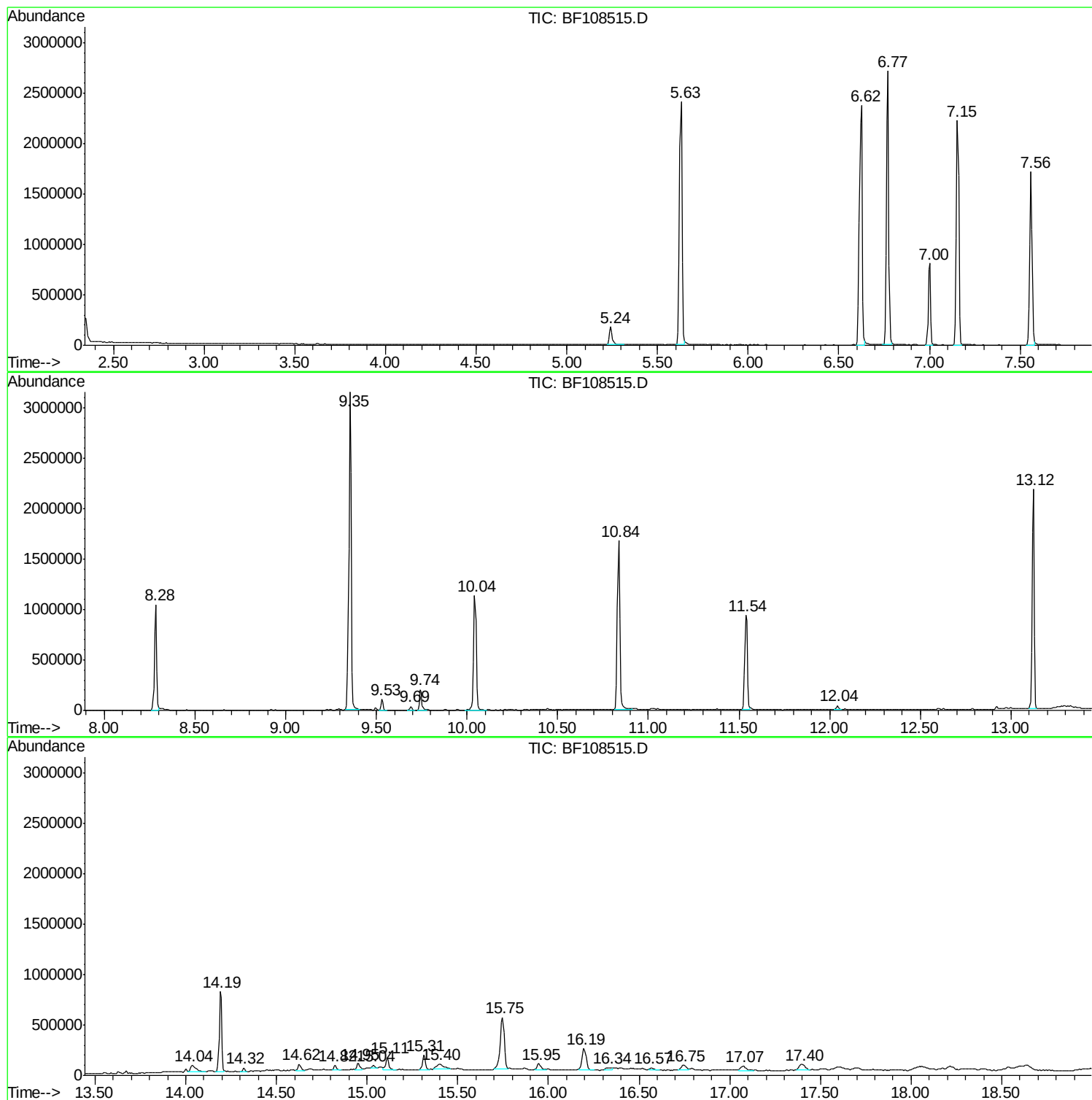
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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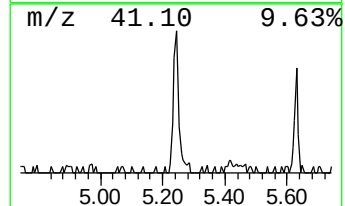
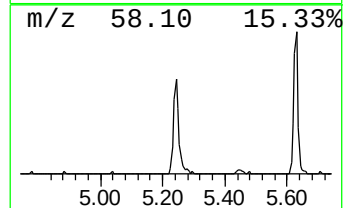
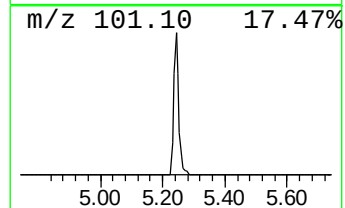
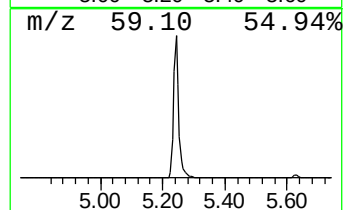
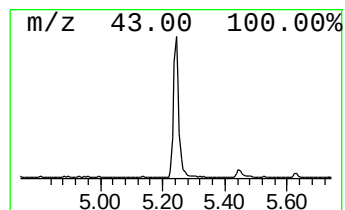
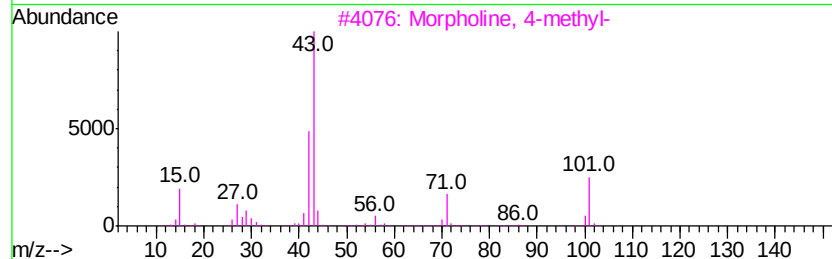
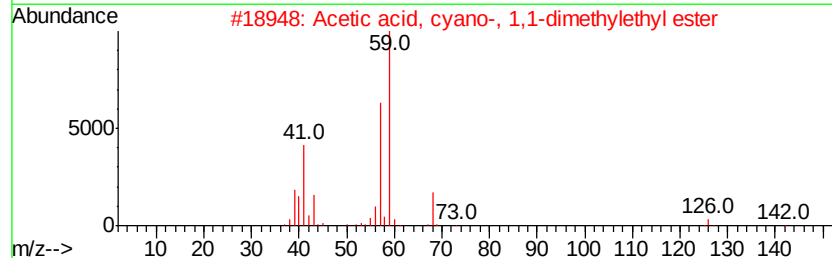
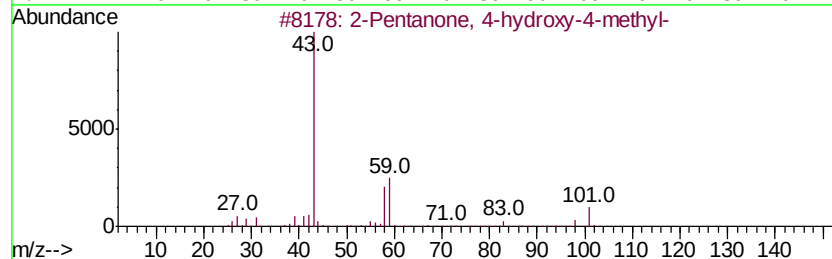
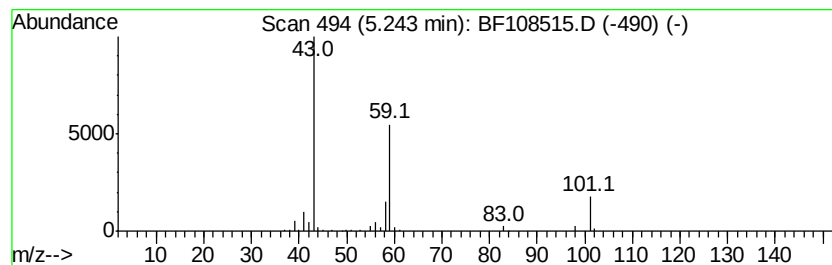
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.24	5.77 ng	207680	1,4-Dichlorobenzene-d4	7.00

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	32
3			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9



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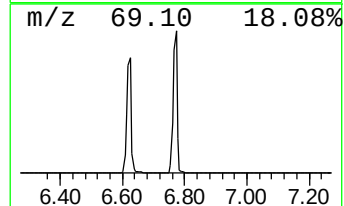
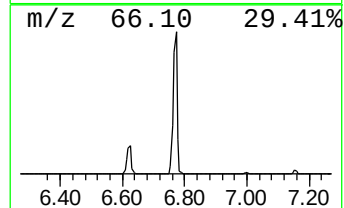
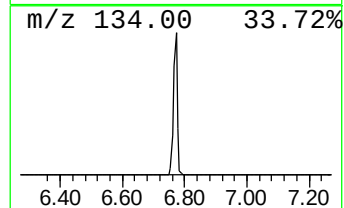
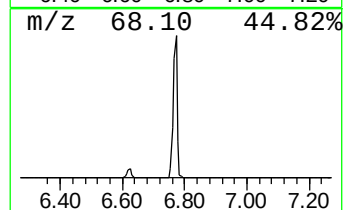
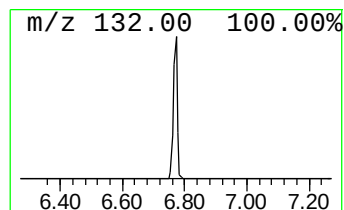
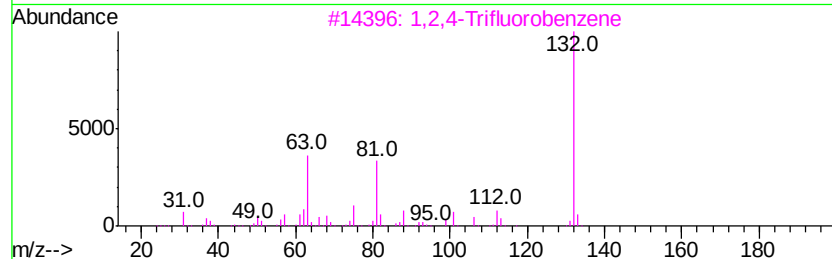
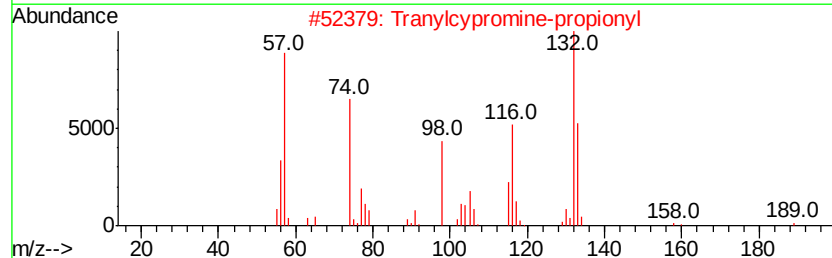
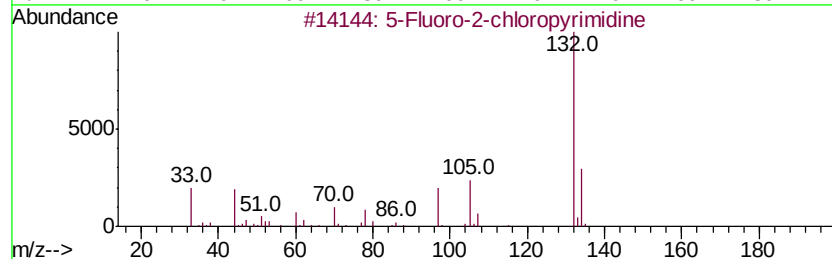
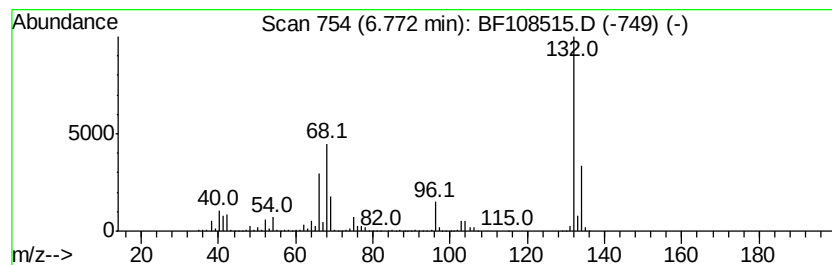
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.77 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	66.86 ng	2407280	1,4-Dichlorobenzene-d4	7.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	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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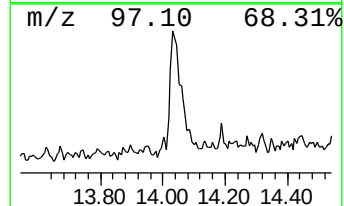
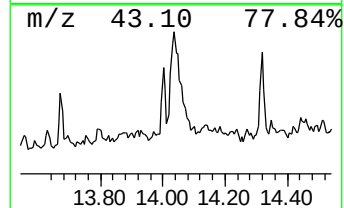
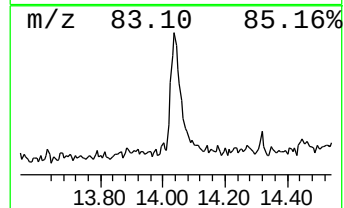
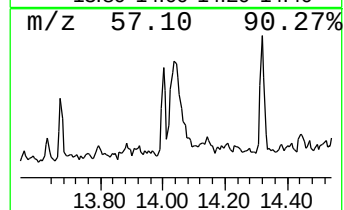
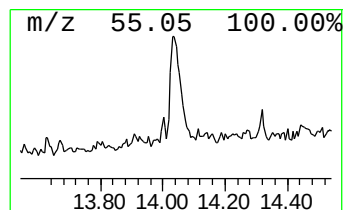
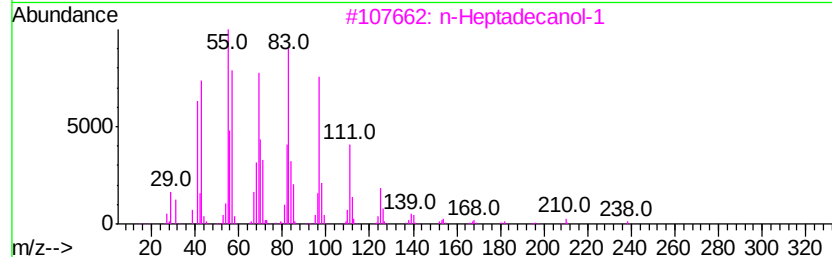
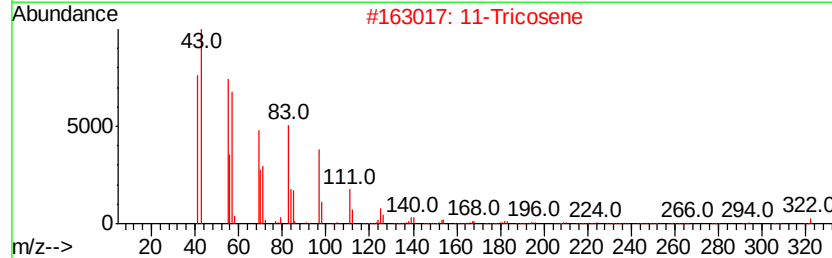
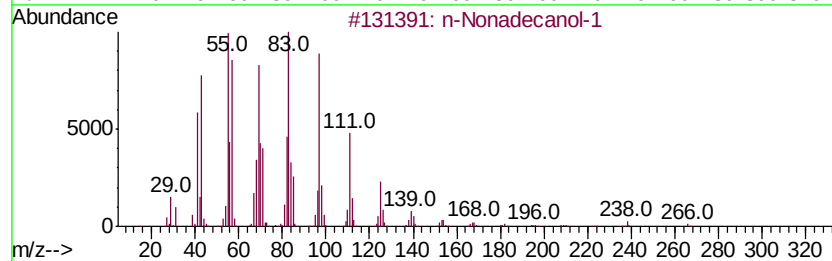
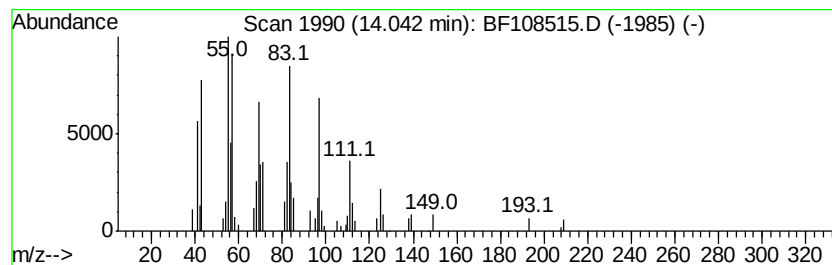
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TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Nonadecanol-1 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.04	3.82 ng	145965	Chrysene-d12		14.19

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Nonadecanol-1	284	C19H40O	001454-84-8	94
2			11-Tricosene	322	C23H46	052078-56-5	91
3			n-Heptadecanol-1	256	C17H36O	001454-85-9	90
4			Pentafluoropropionic acid, dodec...	332	C15H25F5O2	006222-04-4	87
5			Chloroacetic acid, tridecyl ester	276	C15H29ClO2	018277-85-5	87



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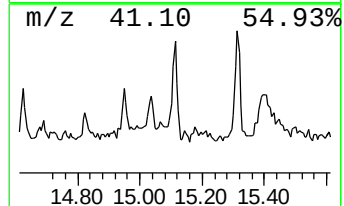
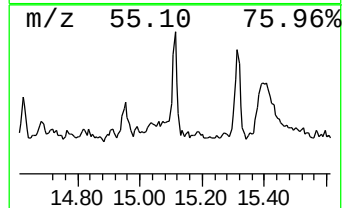
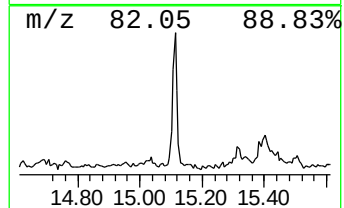
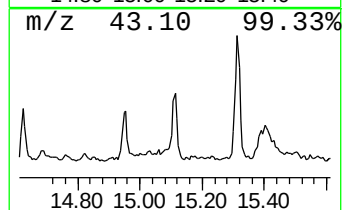
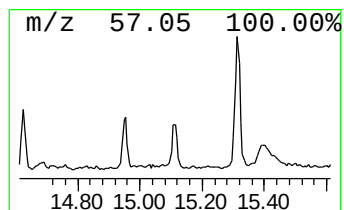
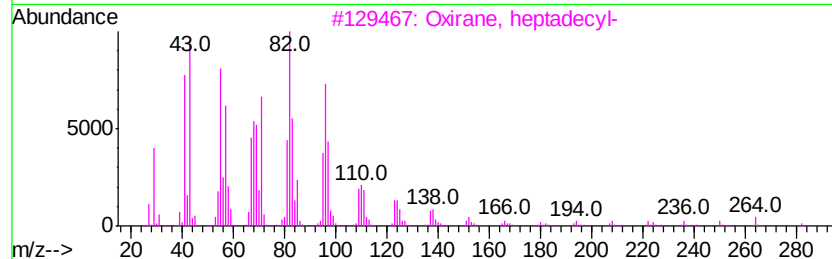
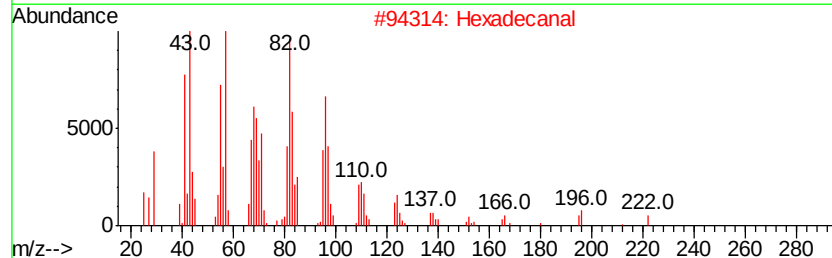
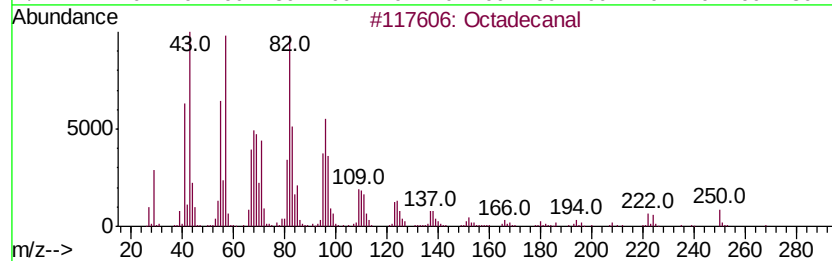
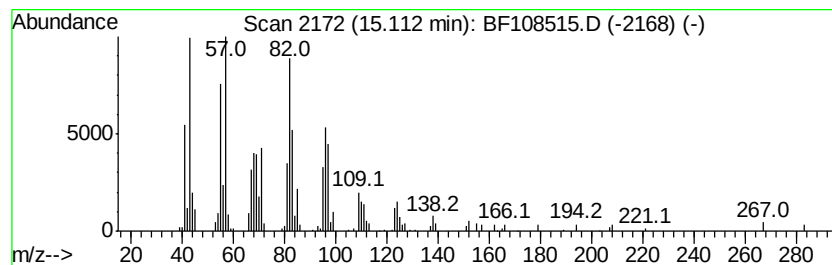
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.11	3.90 ng	151617	Perylene-d12	15.75

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal		268	C18H36O	000638-66-4	91
2	Hexadecanal		240	C16H32O	000629-80-1	91
3	Oxirane, heptadecyl-		282	C19H38O	067860-04-2	90
4	Heptadecanal		254	C17H34O	1000376-70-0	90
5	Oxirane, hexadecyl-		268	C18H36O	007390-81-0	81



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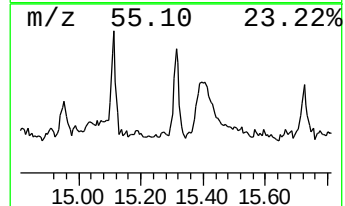
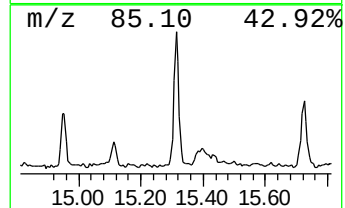
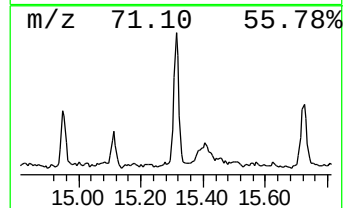
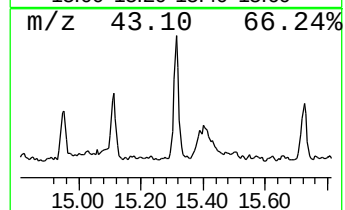
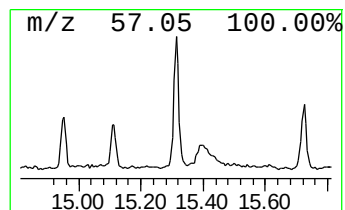
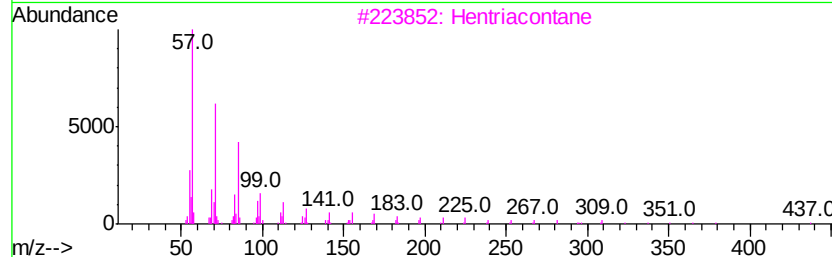
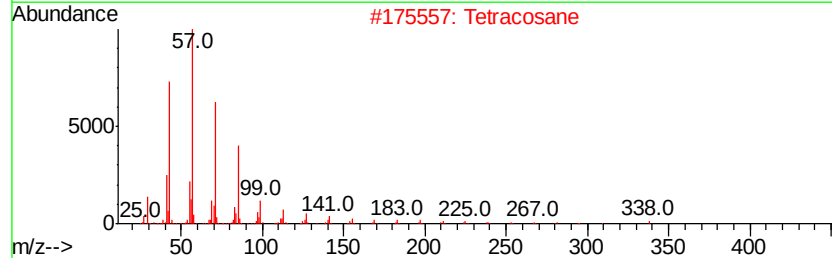
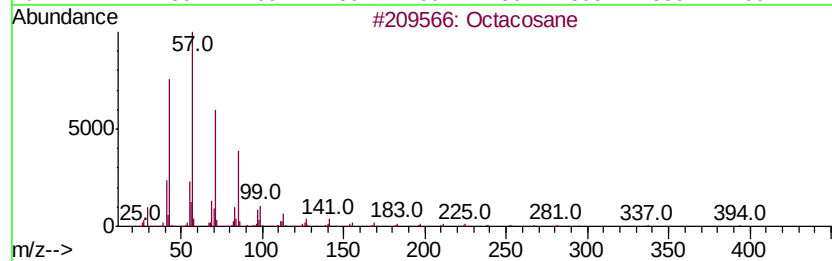
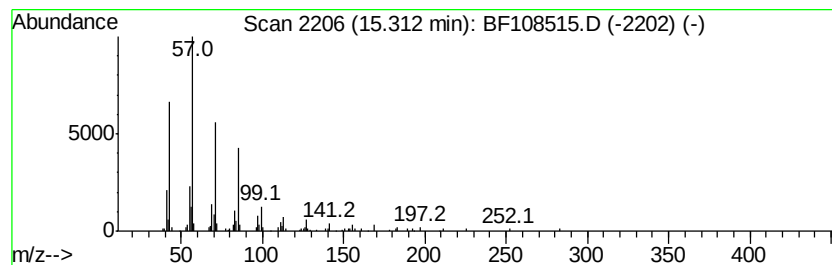
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Peak Number 6 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.31	4.33 ng	168320	Perylene-d12	15.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Tetracosane	338	C24H50	000646-31-1	91
3		Hentriacontane	437	C31H64	000630-04-6	91
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5		Heneicosane	296	C21H44	000629-94-7	91



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Misc :
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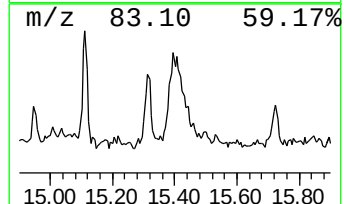
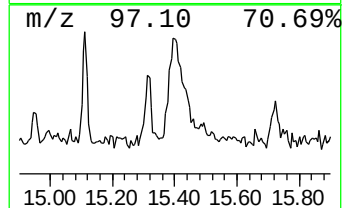
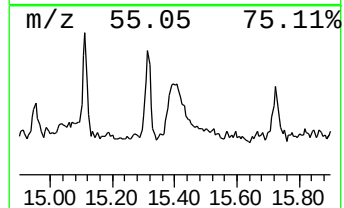
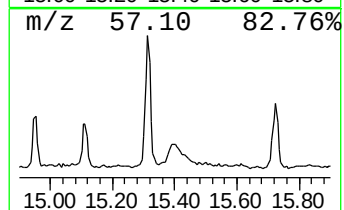
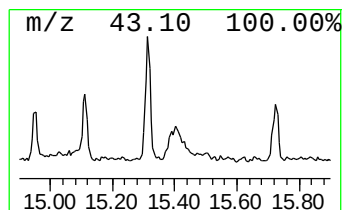
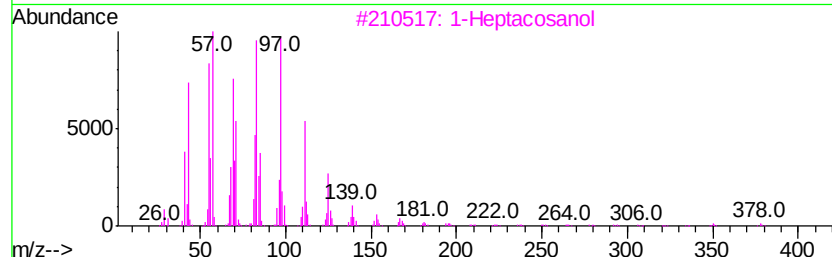
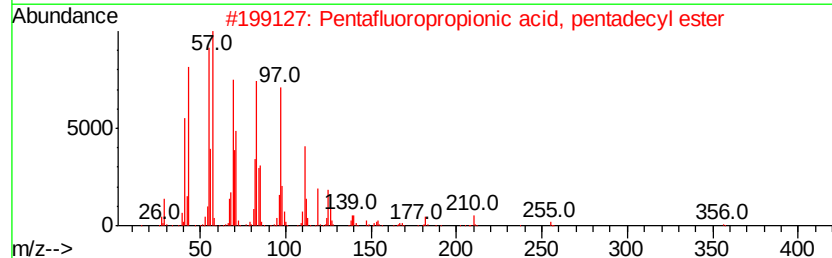
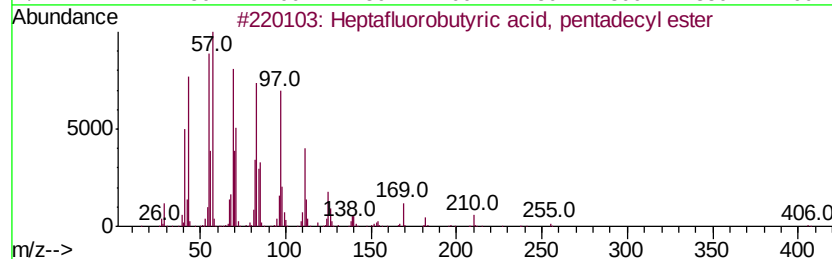
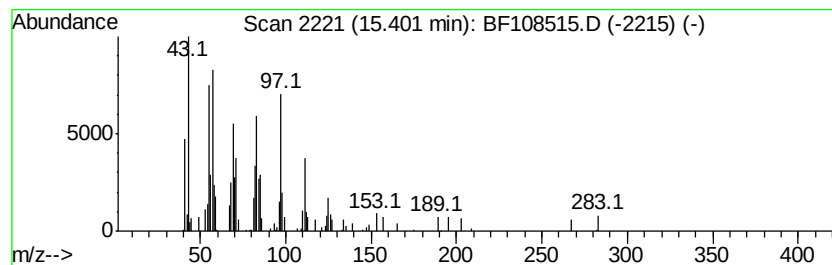
Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptafluorobutyric acid, pe... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.40	3.98 ng	154843	Perylene-d12	15.75
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Heptafluorobutyric acid, pentade...	424 C19H31F7O2	959261-23-5 93
2		Pentafluoropropionic acid, penta...	374 C18H31F5O2	959092-08-1 93
3		1-Heptacosanol	396 C27H56O	002004-39-9 91
4		2-Chloropropionic acid, pentade...	318 C18H35ClO2	1000292-44-1 91
5		Dichloroacetic acid, heptadecyl ...	366 C19H36Cl2O2	1000282-98-2 90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108515.D
Acq On : 27 Aug 2018 17:21
Operator : JU/SJ
Sample : J4538-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

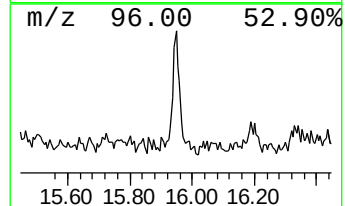
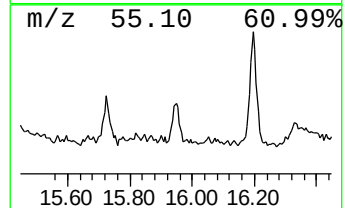
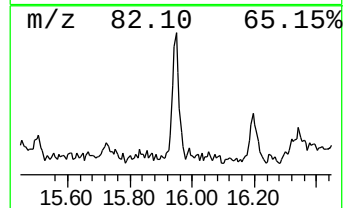
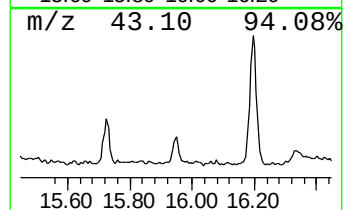
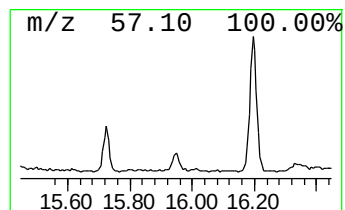
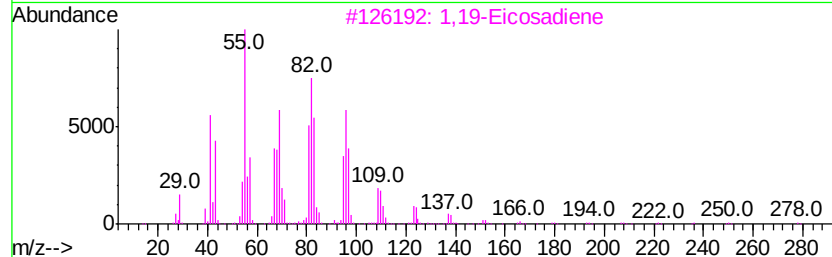
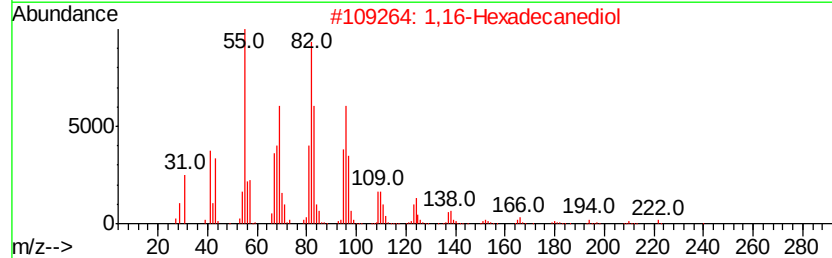
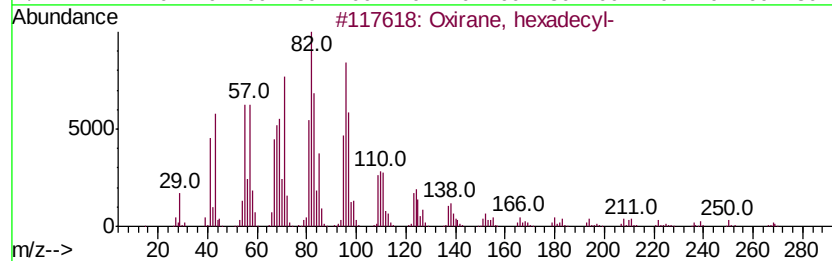
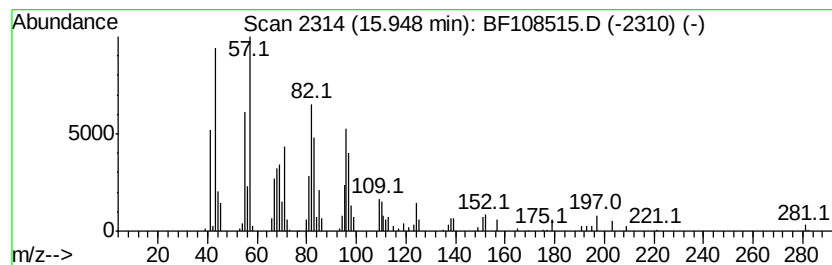
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Oxirane, hexadecyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.95	2.10 ng	81503	Perylene-d12	15.75
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Oxirane, hexadecyl-	268 C18H36O	007390-81-0 90
2		1,16-Hexadecanediol	258 C16H34O2	007735-42-4 58
3		1,19-Eicosadiene	278 C20H38	014811-95-1 58
4		Oxirane, heptadecyl-	282 C19H38O	067860-04-2 49
5		Dodecane, 6-cyclohexyl-	252 C18H36	013151-86-5 47



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108515.D
Acq On : 27 Aug 2018 17:21
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Sample : J4538-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

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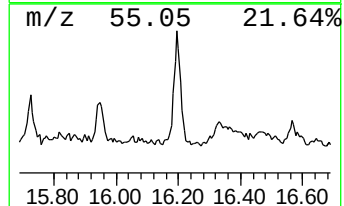
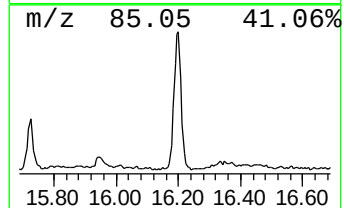
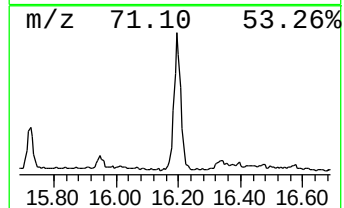
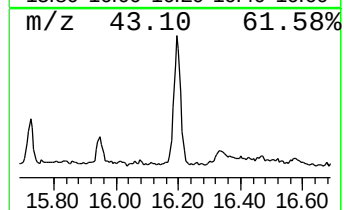
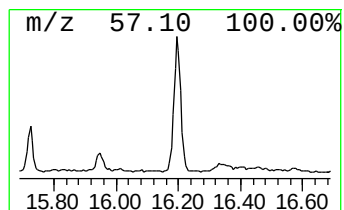
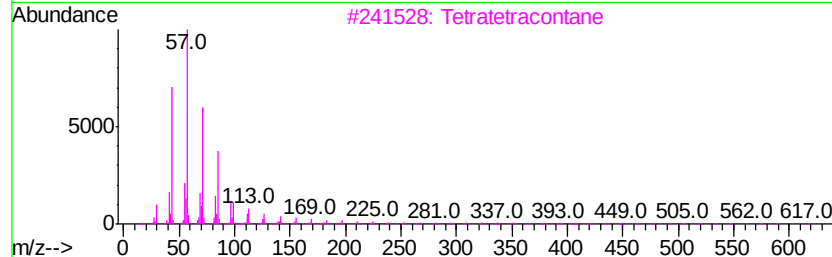
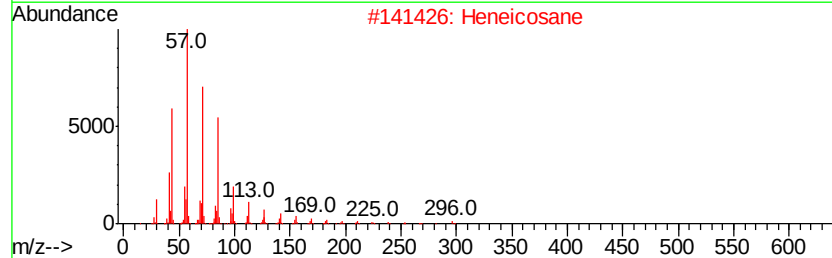
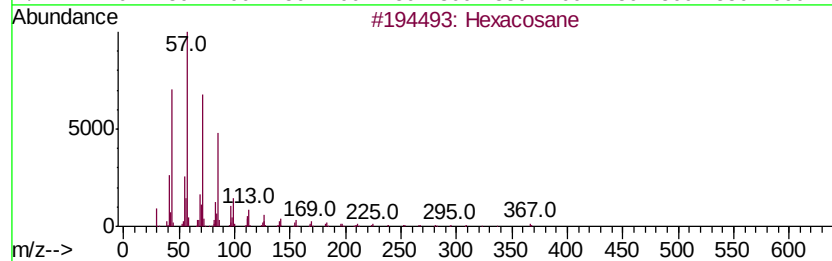
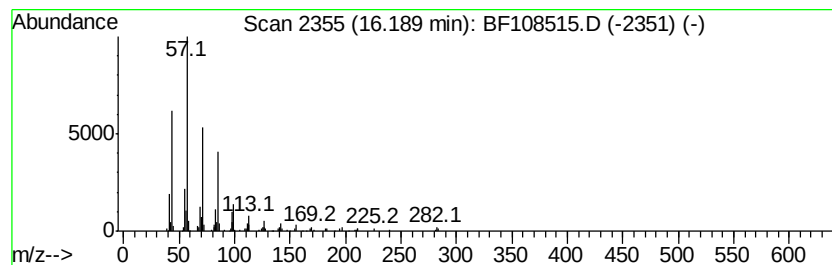
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.19	8.69 ng	337495	Perylene-d12	15.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	94
2		Heneicosane	296	C21H44	000629-94-7	91
3		Tetratetracontane	619	C44H90	007098-22-8	91
4		Hentriacontane	437	C31H64	000630-04-6	91
5		Octacosane	394	C28H58	000630-02-4	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108515.D
Acq On : 27 Aug 2018 17:21
Operator : JU/SJ
Sample : J4538-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VSS2

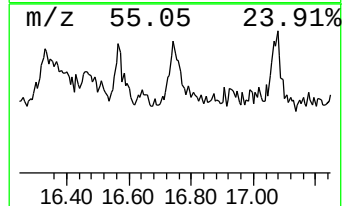
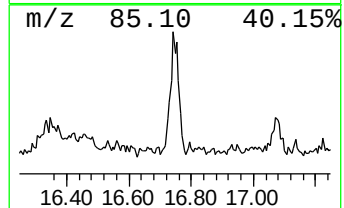
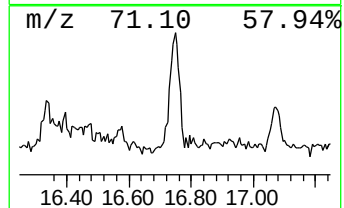
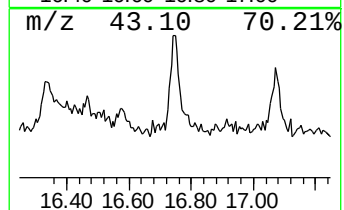
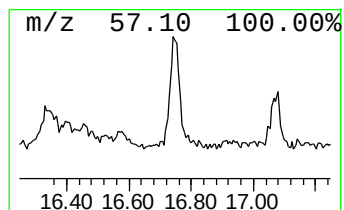
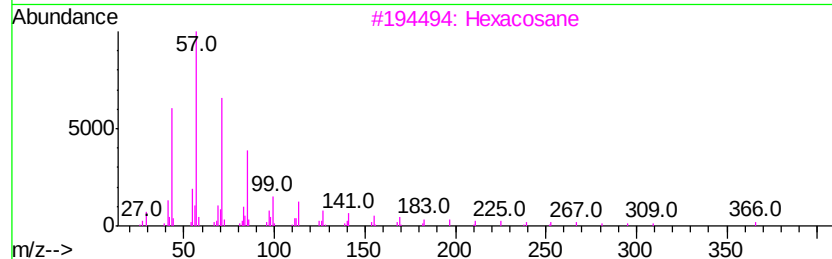
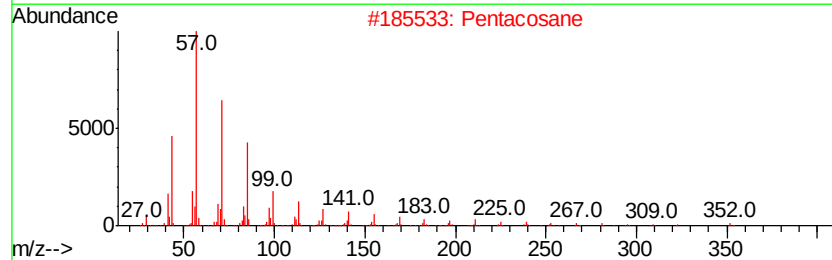
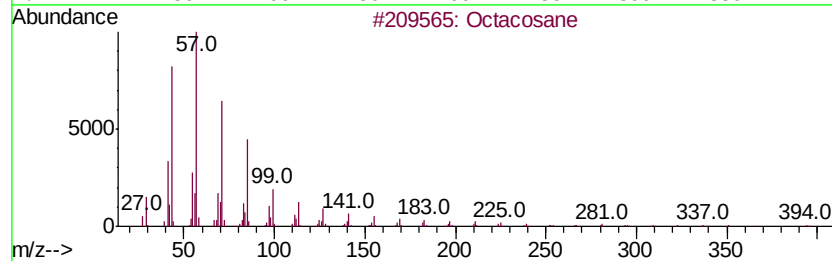
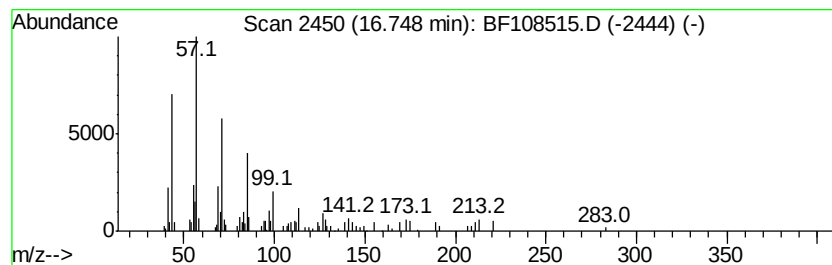
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.75	2.31 ng	89920	Perylene-d12	15.75

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	87
2			Pentacosane	352	C25H52	000629-99-2	86
3			Hexacosane	366	C26H54	000630-01-3	83
4			Heptacosane	380	C27H56	000593-49-7	83
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
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Acq On : 27 Aug 2018 17:21
Operator : JU/SJ
Sample : J4538-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

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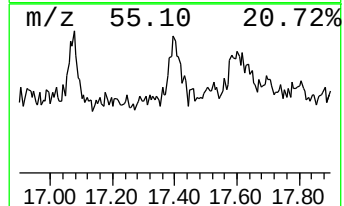
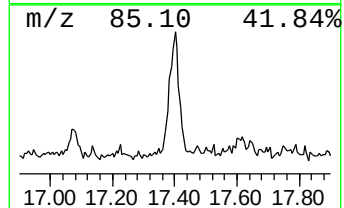
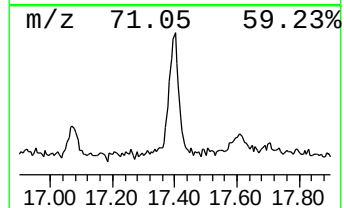
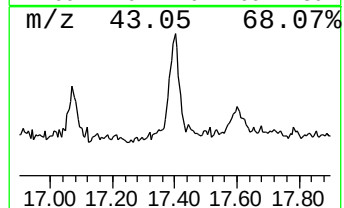
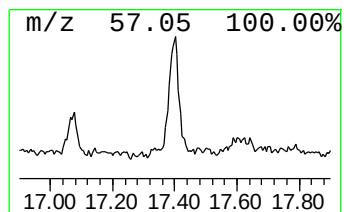
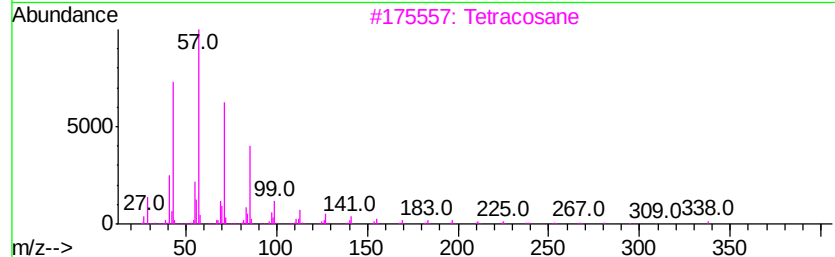
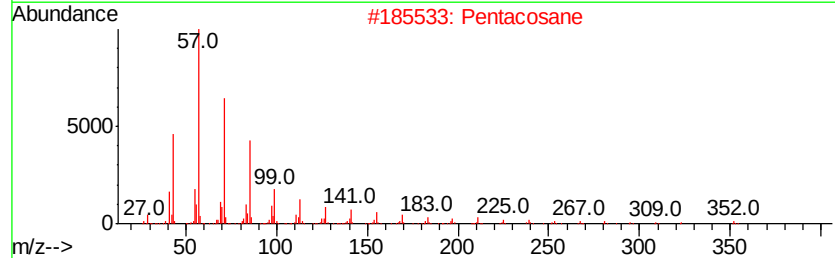
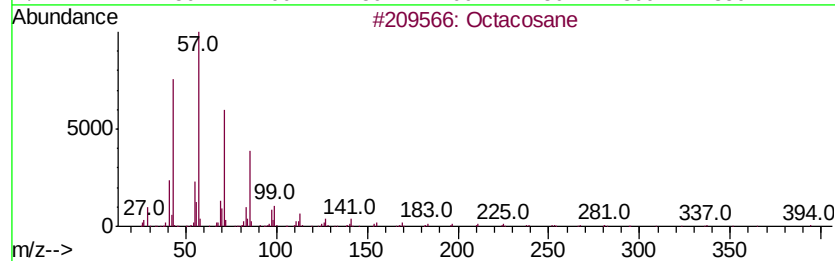
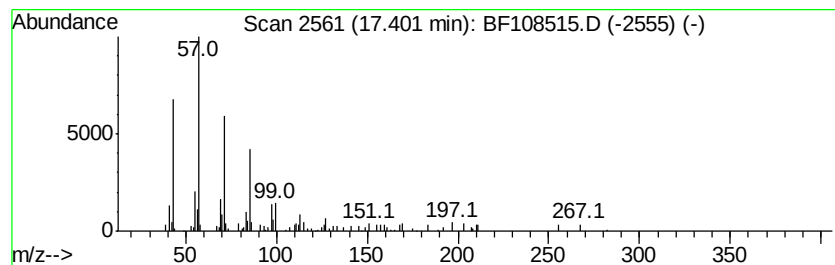
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Pentacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.40	2.90 ng	112667	Perylene-d12	15.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	83
2		Pentacosane	352	C25H52	000629-99-2	83
3		Tetracosane	338	C24H50	000646-31-1	80
4		Hexacosane	366	C26H54	000630-01-3	80
5		Eicosane	282	C20H42	000112-95-8	74



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082718\
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 Acq On : 27 Aug 2018 17:21
 Operator : JU/SJ
 Sample : J4538-02
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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
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unknown6.77	6.77	66.9	ng	2407280	1	7.00	720051	20.0
n-Nonadecanol-1	14.04	3.8	ng	145965	5	14.19	763698	20.0
Octadecanal	15.11	3.9	ng	151617	6	15.75	777184	20.0
Octacosane	15.31	4.3	ng	168320	6	15.75	777184	20.0
Heptafluorobutyri...	15.40	4.0	ng	154843	6	15.75	777184	20.0
Oxirane, hexadecyl-	15.95	2.1	ng	81503	6	15.75	777184	20.0
Hexacosane	16.19	8.7	ng	337495	6	15.75	777184	20.0
Heptacosane	16.75	2.3	ng	89920	6	15.75	777184	20.0
Pentacosane	17.40	2.9	ng	112667	6	15.75	777184	20.0