

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082418\
 Data File : BF108470.D
 Acq On : 24 Aug 2018 18:25
 Operator : JU/SJ
 Sample : J4581-06
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EP1-Q3-B2

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	2.384	3	8	26	rVB	882949	1275417	39.09%	4.072%
2	4.784	412	416	420	rVB	36009	36931	1.13%	0.118%
3	5.254	492	496	505	rVB	113098	148948	4.56%	0.476%
4	5.631	555	560	563	rBV	3039669	2921912	89.55%	9.329%
5	6.625	723	729	741	rBV	2957216	3262854	100.00%	10.418%
6	6.772	749	754	757	rBV	3346560	3173072	97.25%	10.131%
7	6.995	789	792	796	rBV	892610	819808	25.13%	2.618%
8	7.154	815	819	823	rBV	2490015	2213550	67.84%	7.068%
9	7.560	883	888	891	rBV	2068441	2106912	64.57%	6.727%
10	8.284	1006	1011	1014	rBV	1131065	1030316	31.58%	3.290%
11	9.354	1188	1193	1197	rBV	3447610	3116375	95.51%	9.950%
12	9.748	1255	1260	1269	rBV	333771	321423	9.85%	1.026%
13	10.042	1305	1310	1314	rBV2	1378924	1239255	37.98%	3.957%
14	10.836	1440	1445	1458	rBV	2628629	2516904	77.14%	8.036%
15	10.925	1458	1460	1466	rVB	35610	40652	1.25%	0.130%
16	11.536	1560	1564	1568	rBV	1341746	1267766	38.85%	4.048%
17	12.042	1644	1650	1653	rBV	135220	122773	3.76%	0.392%
18	12.078	1653	1656	1662	rVB2	27023	39236	1.20%	0.125%
19	12.754	1768	1771	1775	rVB	44682	43817	1.34%	0.140%
20	12.989	1805	1811	1816	rBV2	59291	85934	2.63%	0.274%
21	13.125	1829	1834	1837	rBV	3329820	2909215	89.16%	9.289%
22	13.330	1862	1869	1873	rBV2	37530	40555	1.24%	0.129%
23	13.672	1923	1927	1930	rBV2	53408	46211	1.42%	0.148%
24	14.001	1980	1983	1987	rVB	65485	54468	1.67%	0.174%
25	14.066	1989	1994	2004	rBV9	30228	91900	2.82%	0.293%
26	14.189	2011	2015	2019	rBV	852154	790884	24.24%	2.525%
27	14.319	2032	2037	2040	rBV2	70344	75033	2.30%	0.240%
28	14.624	2086	2089	2093	rVB	65660	64392	1.97%	0.206%
29	14.942	2139	2143	2152	rVB2	110939	170174	5.22%	0.543%
30	15.036	2155	2159	2164	rVB	175774	189130	5.80%	0.604%
31	15.313	2203	2206	2213	rVB	75516	88648	2.72%	0.283%
32	15.742	2271	2279	2289	rVB	524954	820633	25.15%	2.620%
33	16.195	2351	2356	2363	rVB	73172	122629	3.76%	0.392%
34	16.742	2445	2449	2458	rVB2	40928	72387	2.22%	0.231%

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Instrument :
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ClientSampleId :
EP1-Q3-B2

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-BF080818.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

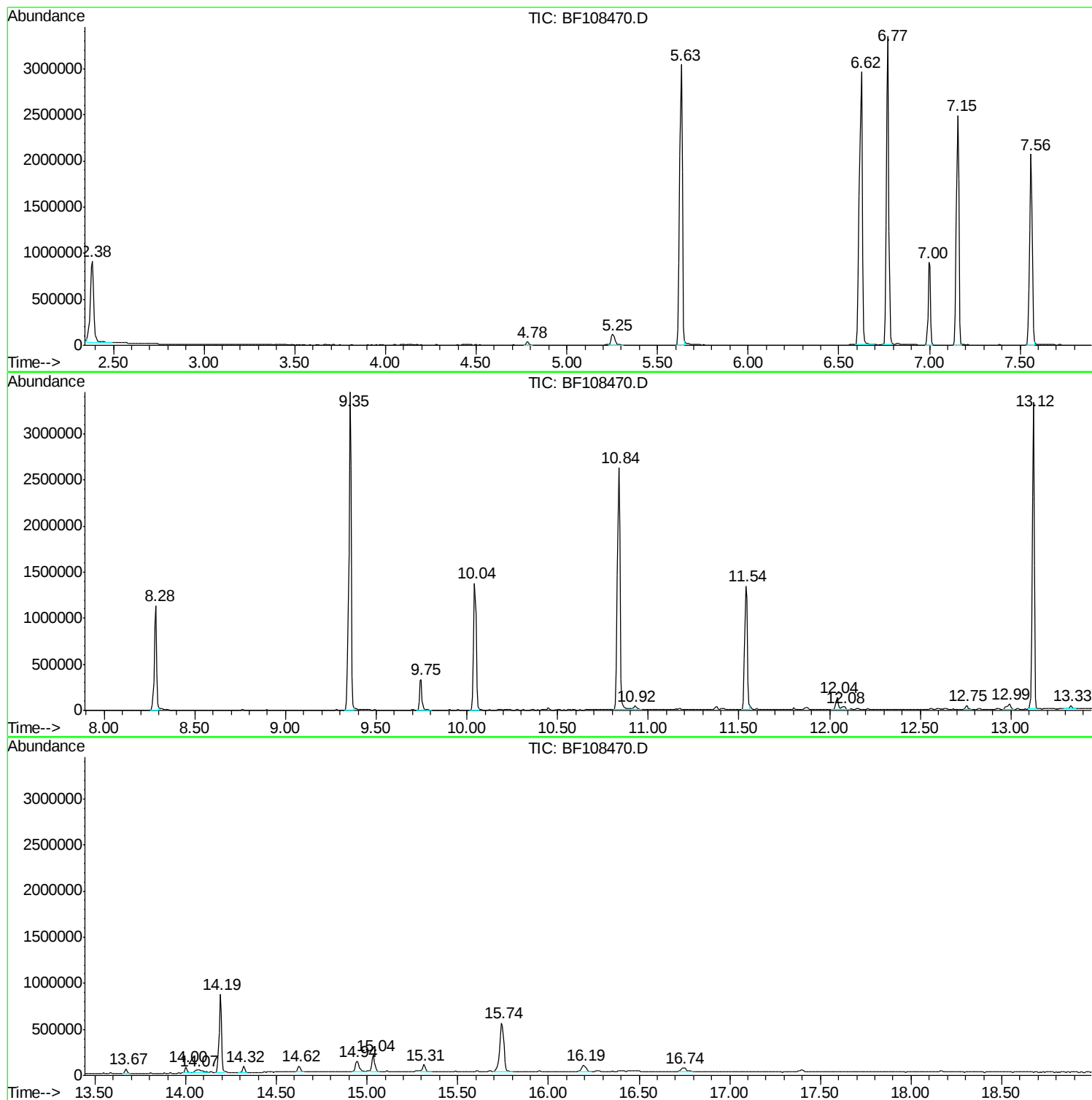
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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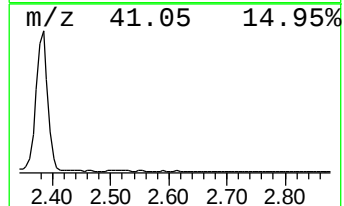
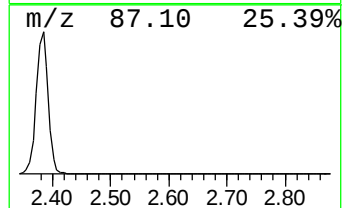
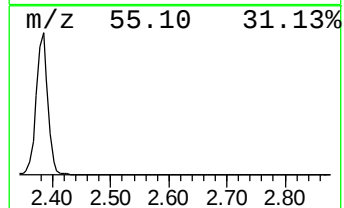
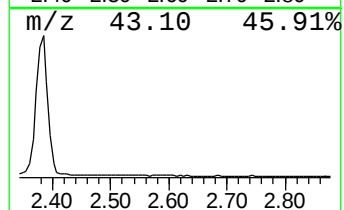
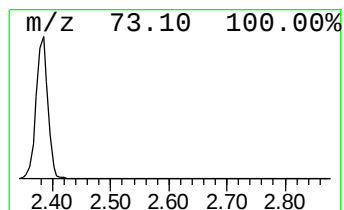
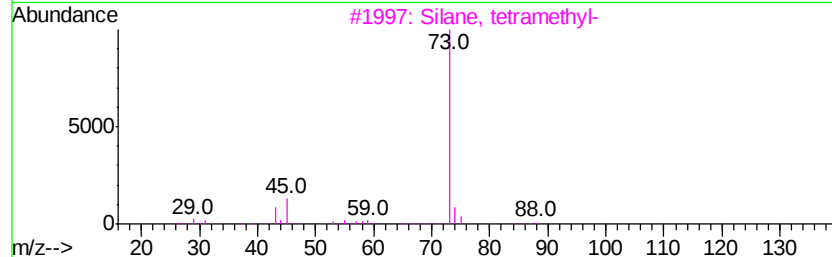
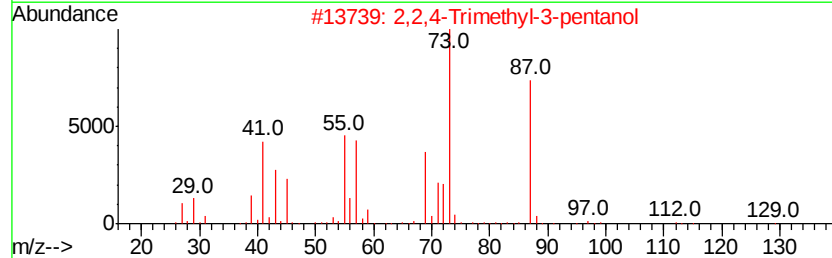
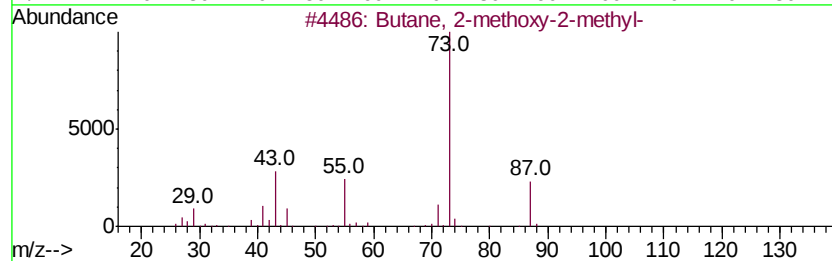
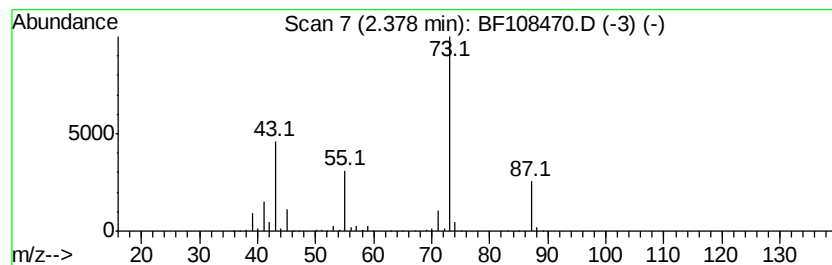
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.38	31.12 ng	1275420	1,4-Dichlorobenzene-d4	7.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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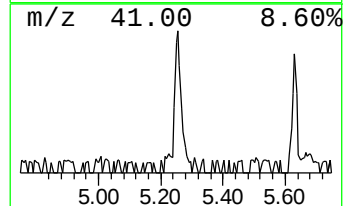
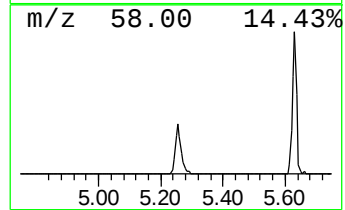
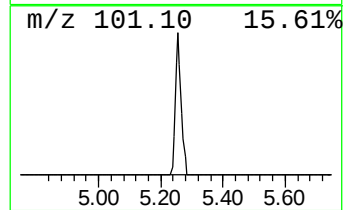
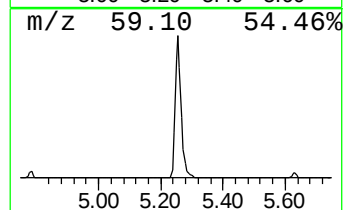
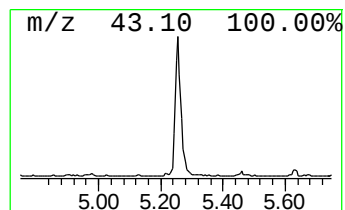
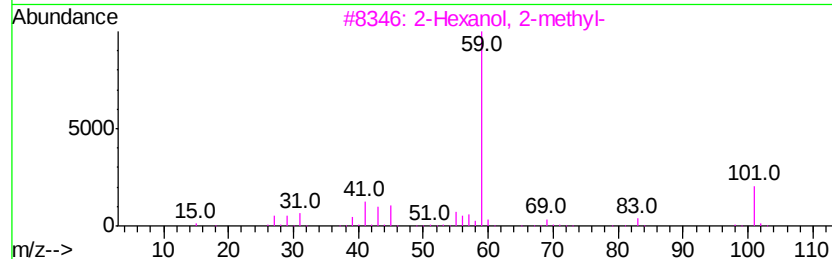
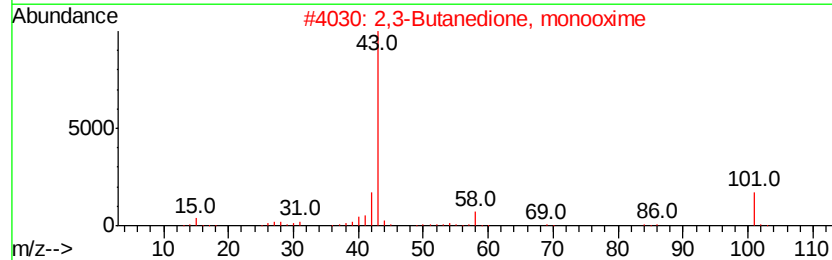
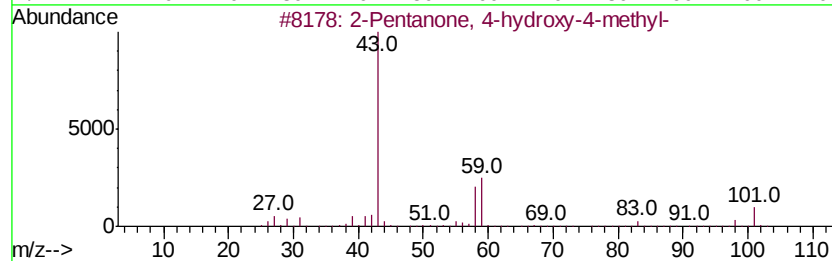
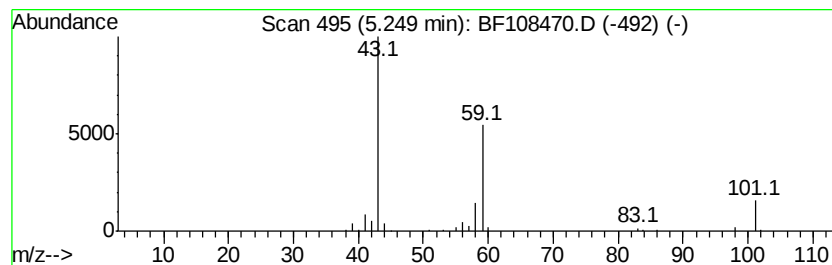
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.25	3.63 ng	148948	1,4-Dichlorobenzene-d4	7.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9



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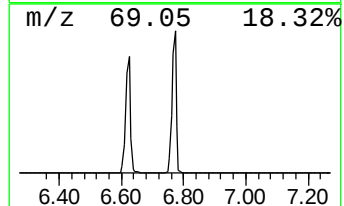
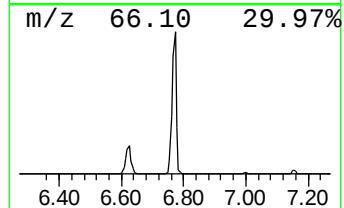
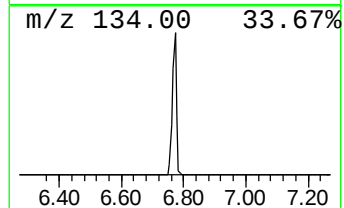
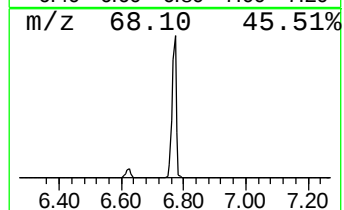
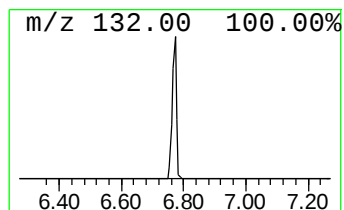
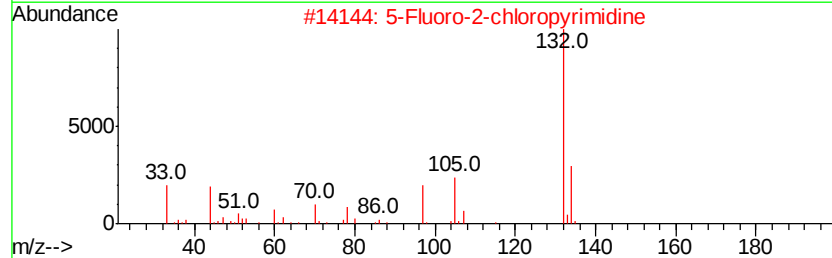
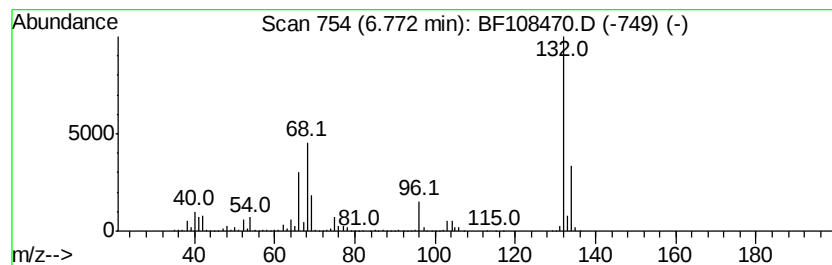
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.77 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	77.41 ng	3173070	1,4-Dichlorobenzene-d4	7.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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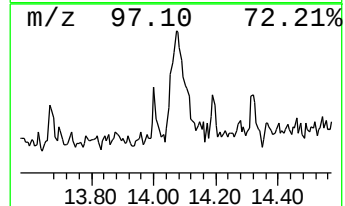
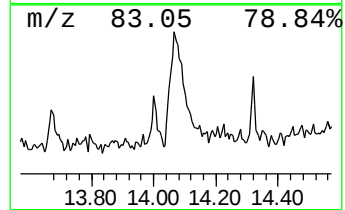
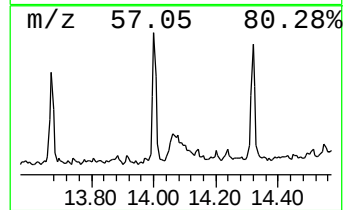
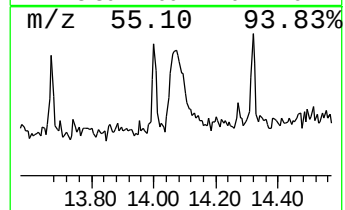
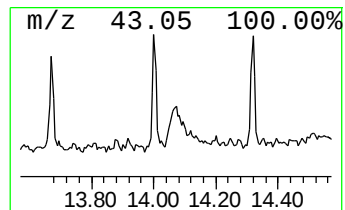
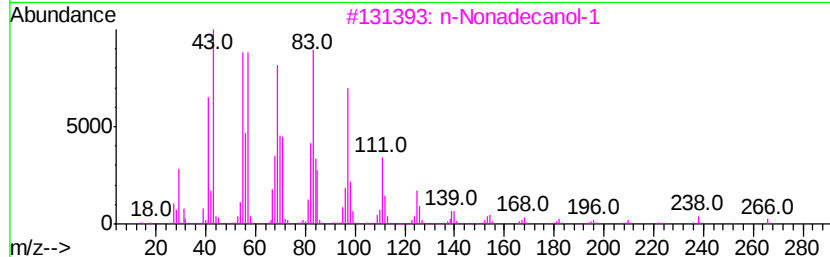
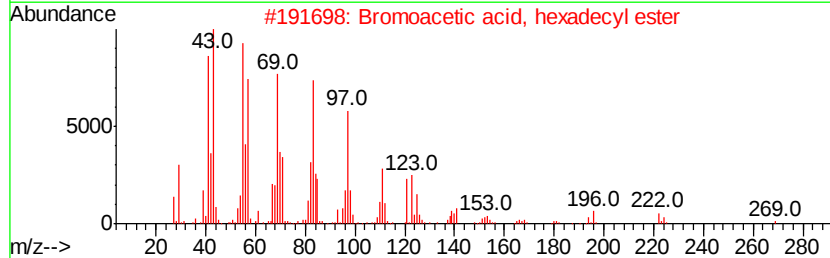
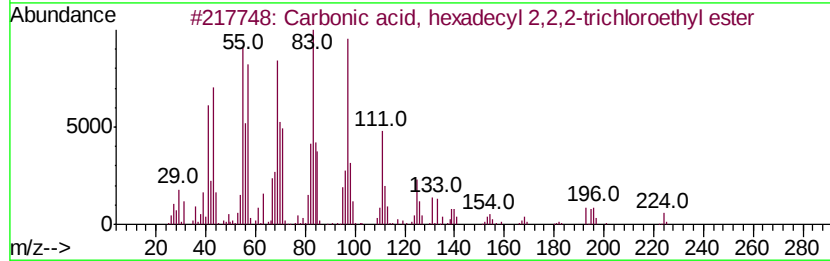
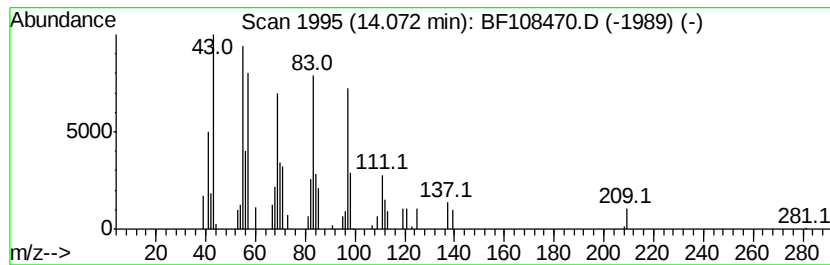
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Carbonic acid, hexadecyl 2,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.07	2.32 ng	91900	Chrysene-d12	14.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Carbonic acid, hexadecyl 2,2,2-t...	416	C19H35Cl3O3	1000314-56-2	91
2		Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	90
3		n-Nonadecanol-1	284	C19H40O	001454-84-8	90
4		Dichloroacetic acid, tridecyl ester	310	C15H28Cl2O2	1000280-48-3	90
5		Bromoacetic acid, tetradecyl ester	334	C16H31BrO2	018992-01-3	86



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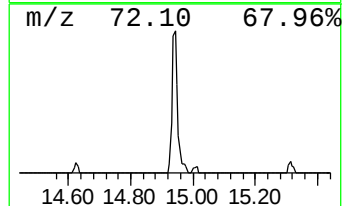
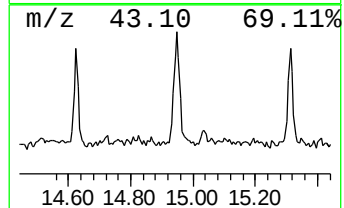
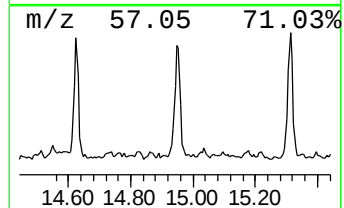
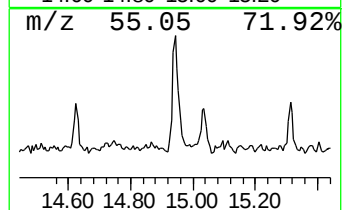
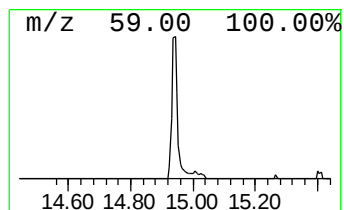
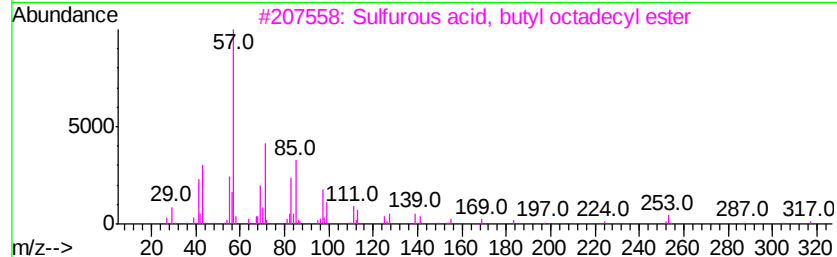
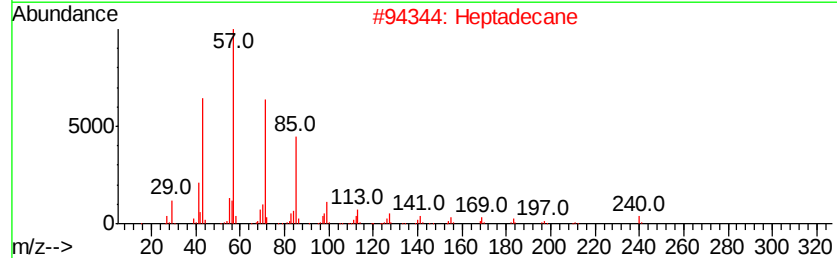
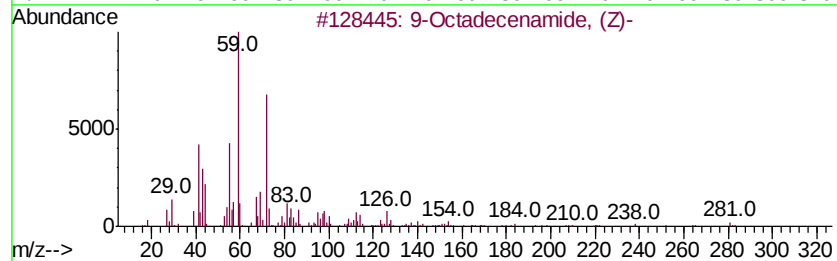
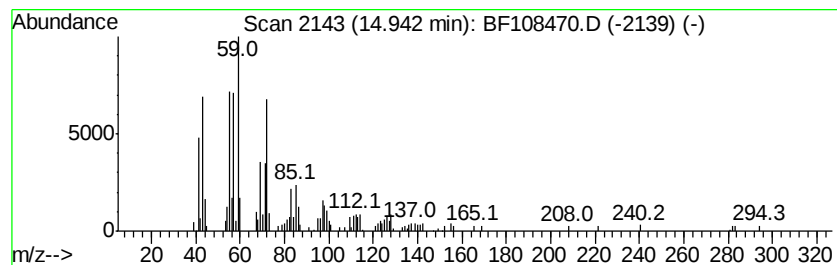
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.94	4.30 ng	170174	Chrysene-d12	14.19

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	93
2		Heptadecane	240	C17H36	000629-78-7	53
3		Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	30
4		Eicosane	282	C20H42	000112-95-8	25
5		Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	25



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ClientSampleId :
EP1-Q3-B2

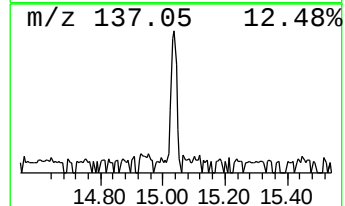
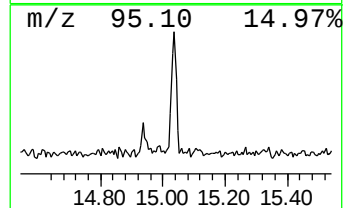
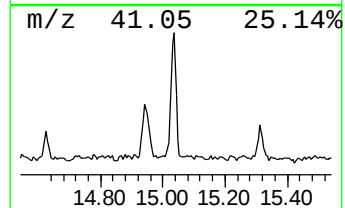
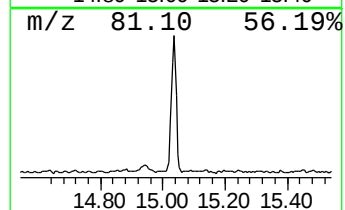
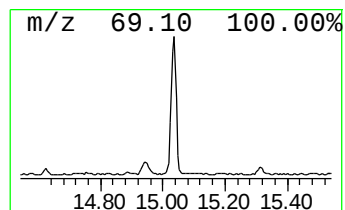
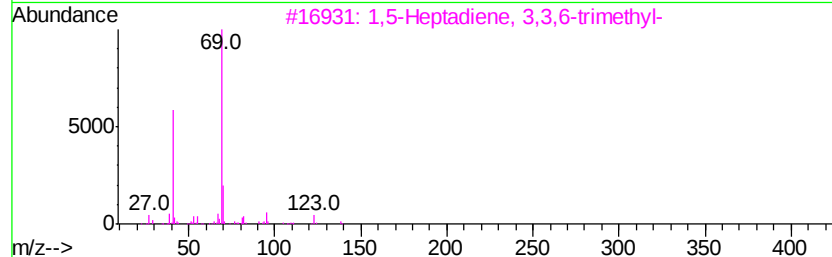
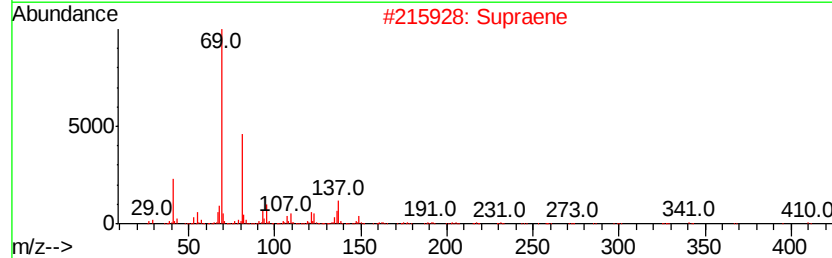
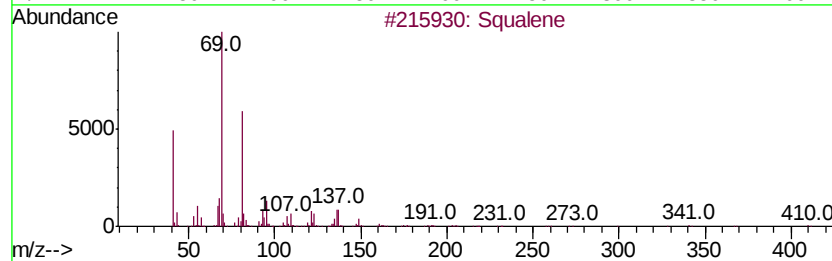
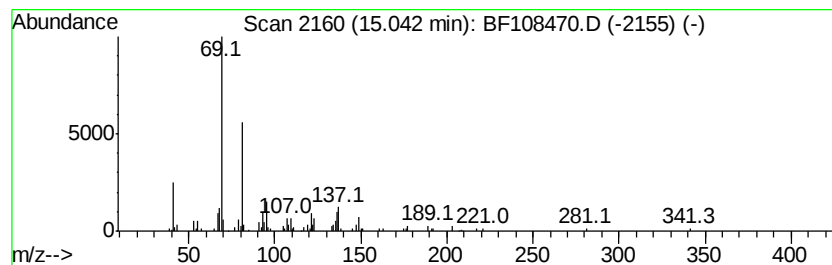
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.04	4.61 ng	189130	Perylene-d12	15.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	87
3		1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	52
4		2,6-Octadiene, 2,7-dimethyl-	138	C10H18	016736-42-8	50
5		1,5-Heptadiene, 3,4-dimethyl-	124	C9H16	1000061-77-9	47



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082418\
Data File : BF108470.D
Acq On : 24 Aug 2018 18:25
Operator : JU/SJ
Sample : J4581-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP1-Q3-B2

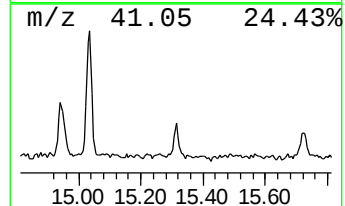
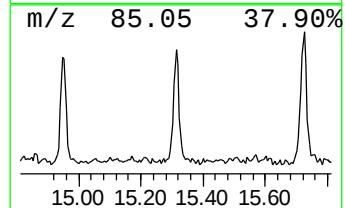
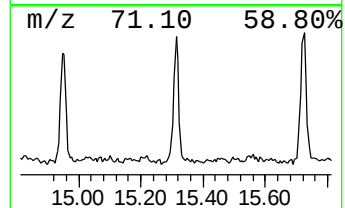
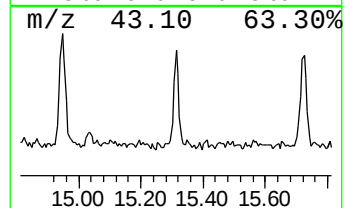
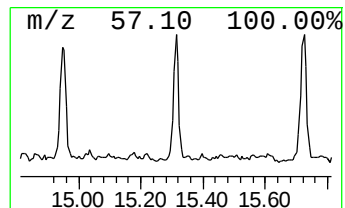
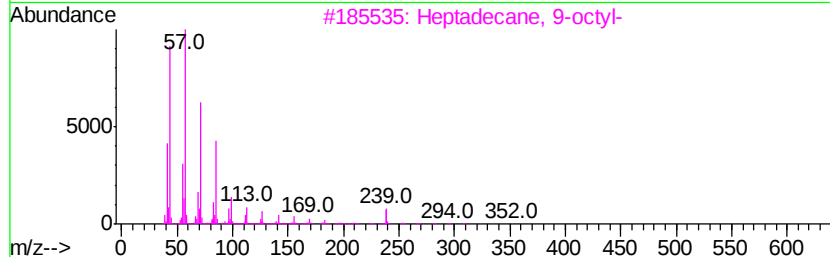
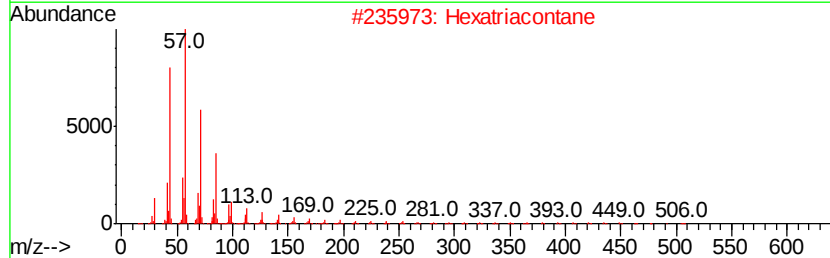
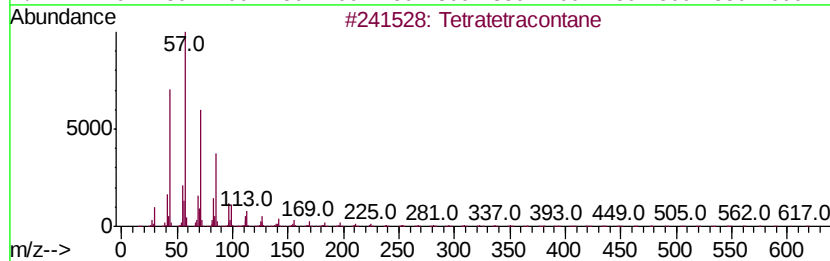
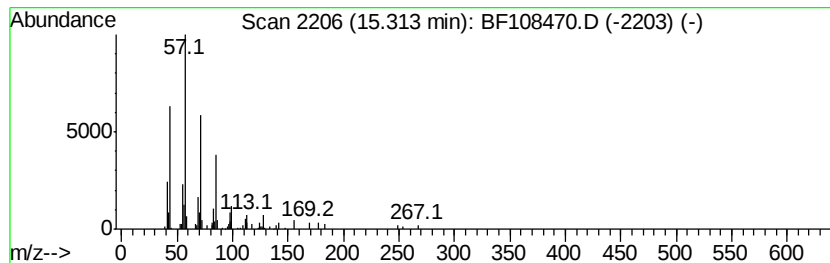
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetratetracontane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.31	2.16 ng	88648	Perylene-d12	15.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetratetracontane	619	C44H90	007098-22-8	90
2		Hexatriacontane	507	C36H74	000630-06-8	90
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
4		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87
5		Octacosane	394	C28H58	000630-02-4	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082418\
Data File : BF108470.D
Acq On : 24 Aug 2018 18:25
Operator : JU/SJ
Sample : J4581-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP1-Q3-B2

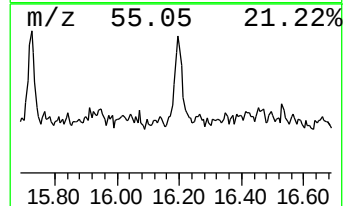
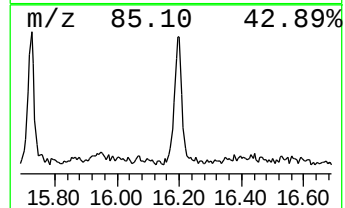
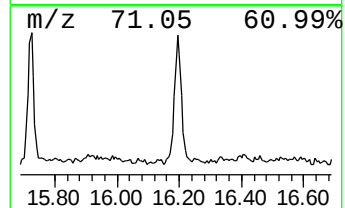
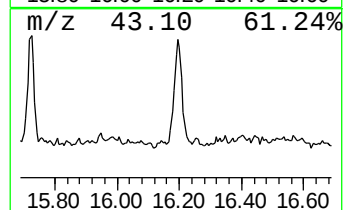
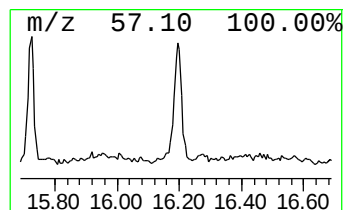
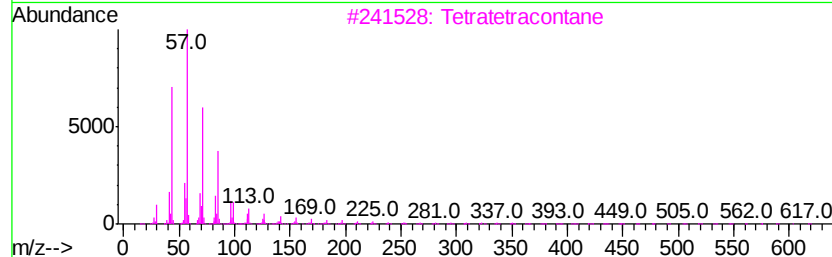
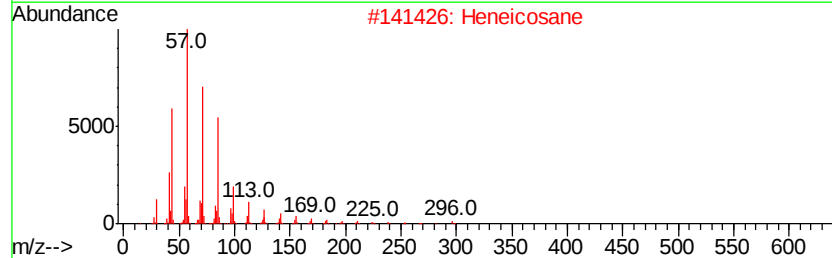
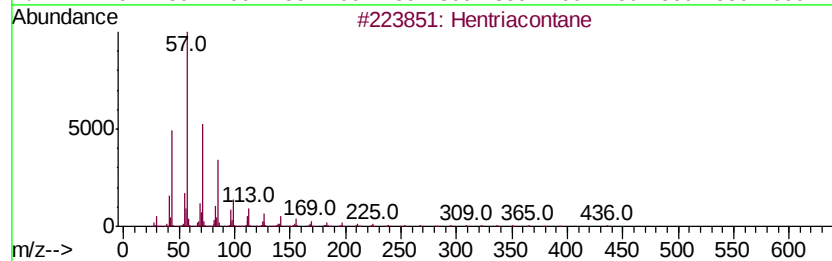
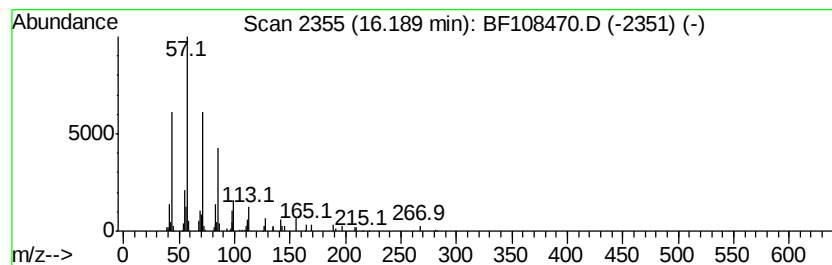
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hentriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.19	2.99 ng	122629	Perylene-d12	15.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hentriacontane	437	C31H64	000630-04-6	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Tetratetracontane	619	C44H90	007098-22-8	91
4		Octacosane	394	C28H58	000630-02-4	91
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082418\
Data File : BF108470.D
Acq On : 24 Aug 2018 18:25
Operator : JU/SJ
Sample : J4581-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP1-Q3-B2

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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2-Pentanone, 4-hy...	5.25	3.6	ng	148948	1	7.00	819808	20.0
unknown6.77	6.77	77.4	ng	3173070	1	7.00	819808	20.0
Carbonic acid, he...	14.07	2.3	ng	91900	5	14.19	790884	20.0
9-Octadecenamide,...	14.94	4.3	ng	170174	5	14.19	790884	20.0
Squalene	15.04	4.6	ng	189130	6	15.74	820633	20.0
Tetratetracontane	15.31	2.2	ng	88648	6	15.74	820633	20.0
Hentriacontane	16.19	3.0	ng	122629	6	15.74	820633	20.0