

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081418\
 Data File : BF108144.D
 Acq On : 14 Aug 2018 15:00
 Operator : JU/SJ
 Sample : J4447-36
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-1-10

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	2.378	3	7	17	rVB	446886	624673	15.84%	1.733%
2	5.266	492	498	507	rVB	672844	828870	21.01%	2.299%
3	5.648	558	563	566	rBV	4089359	3859406	97.85%	10.705%
4	6.637	726	731	734	rBV	3818308	3944259	100.00%	10.940%
5	6.790	752	757	760	rBV	4275567	3922510	99.45%	10.880%
6	7.019	792	796	800	rVB	1301957	1007268	25.54%	2.794%
7	7.178	819	823	826	rBV	3347963	2875397	72.90%	7.975%
8	7.578	886	891	894	rBV	2487098	2434926	61.73%	6.754%
9	8.301	1010	1014	1018	rBV	1295241	1126164	28.55%	3.124%
10	9.378	1192	1197	1200	rBV	3498135	3303004	83.74%	9.161%
11	9.766	1259	1263	1266	rBV	457579	376426	9.54%	1.044%
12	9.972	1295	1298	1302	rVB2	51316	48347	1.23%	0.134%
13	10.066	1310	1314	1318	rVB	1251570	1043117	26.45%	2.893%
14	10.472	1380	1383	1386	rVB2	53725	49192	1.25%	0.136%
15	10.695	1417	1421	1424	rBV	46840	50471	1.28%	0.140%
16	10.860	1444	1449	1452	rBV	2292739	2185969	55.42%	6.063%
17	10.960	1461	1466	1475	rVB	101931	155772	3.95%	0.432%
18	11.430	1543	1546	1549	rVB2	47159	45026	1.14%	0.125%
19	11.560	1564	1568	1571	rBV	1290991	1081879	27.43%	3.001%
20	11.895	1622	1625	1628	rVB	48003	51011	1.29%	0.141%
21	12.060	1650	1653	1657	rBV	87593	89697	2.27%	0.249%
22	12.101	1657	1660	1665	rVB	40634	61022	1.55%	0.169%
23	13.013	1810	1815	1821	rBV4	62310	122295	3.10%	0.339%
24	13.148	1834	1838	1841	rBV	3935793	3555129	90.13%	9.861%
25	13.354	1871	1873	1876	rVB2	58543	52715	1.34%	0.146%
26	13.701	1929	1932	1934	rBV2	81839	69649	1.77%	0.193%
27	14.030	1984	1988	1993	rBV	440485	480037	12.17%	1.331%
28	14.213	2016	2019	2023	rBV	1188656	1138767	28.87%	3.159%
29	14.348	2039	2042	2046	rBV2	162765	157215	3.99%	0.436%
30	14.654	2092	2094	2102	rBV3	150060	235750	5.98%	0.654%
31	14.983	2148	2150	2153	rVB	122373	114916	2.91%	0.319%
32	15.354	2210	2213	2217	rVB	130879	145714	3.69%	0.404%
33	15.777	2281	2285	2290	rVB	577528	816734	20.71%	2.265%

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ClientSampleId :
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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

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

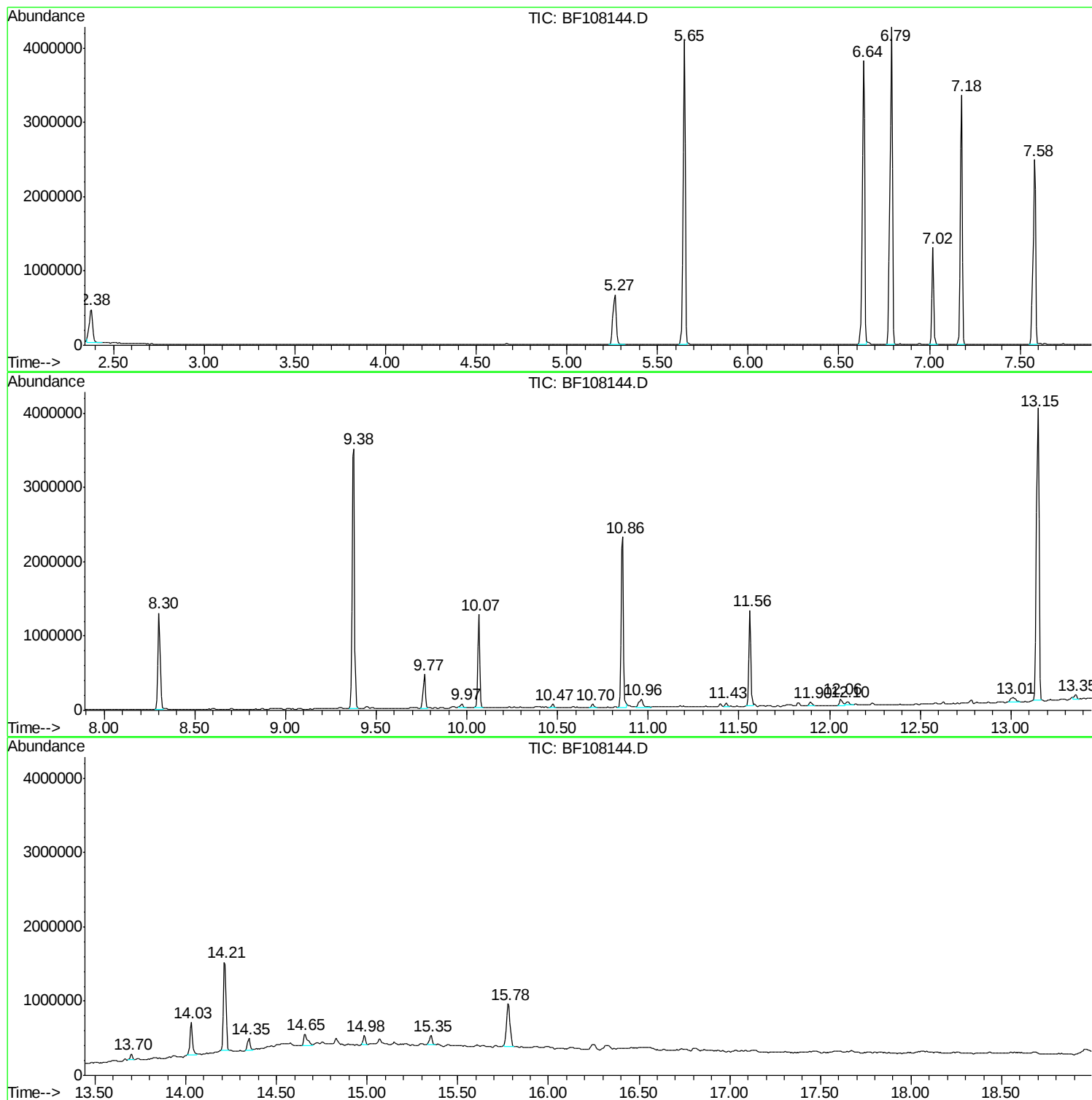
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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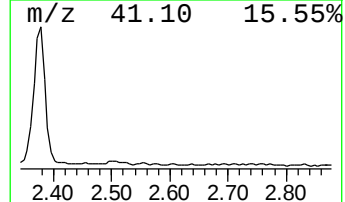
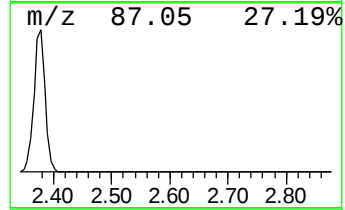
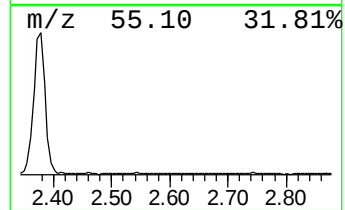
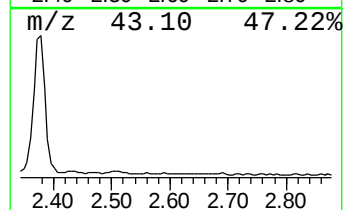
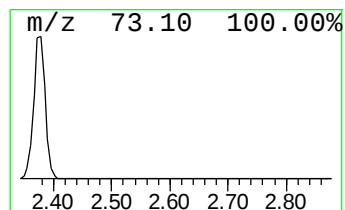
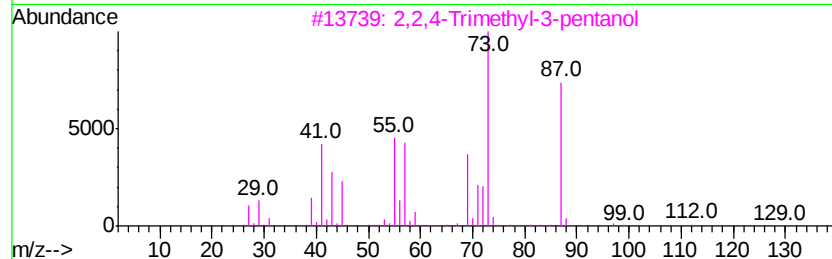
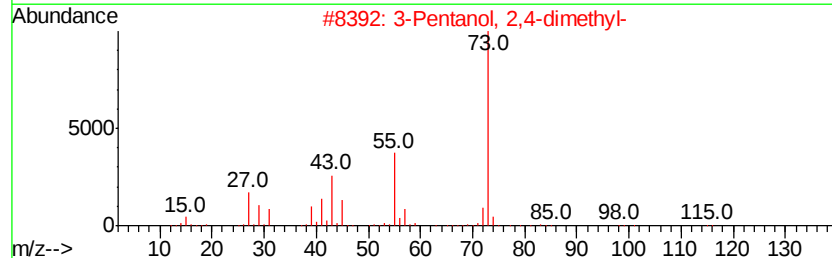
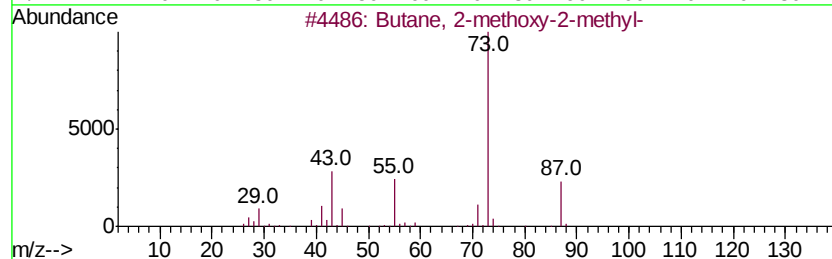
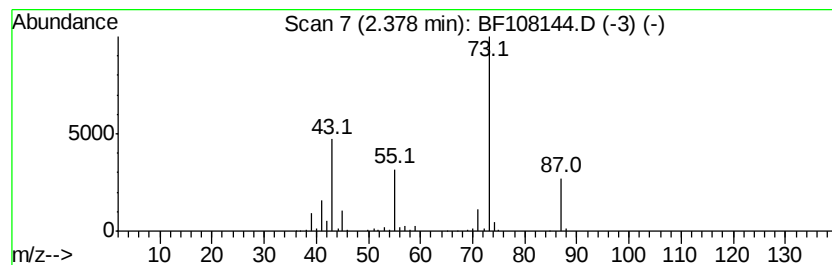
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.38	12.40 ng	624673	1,4-Dichlorobenzene-d4	7.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23



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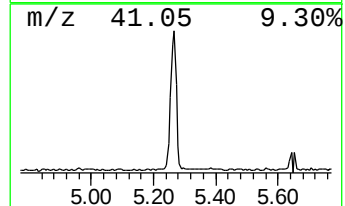
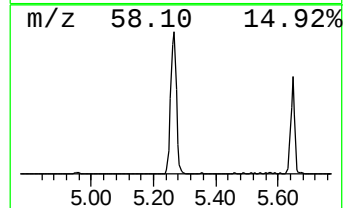
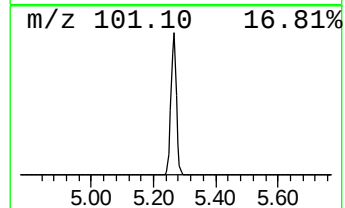
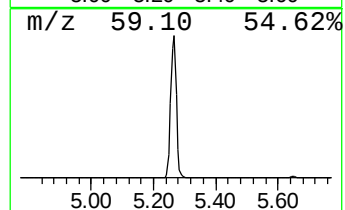
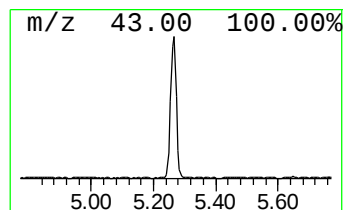
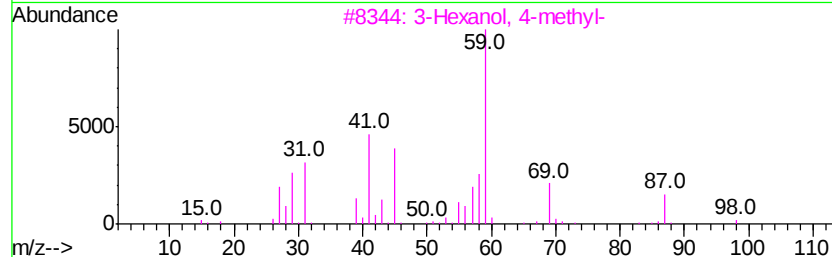
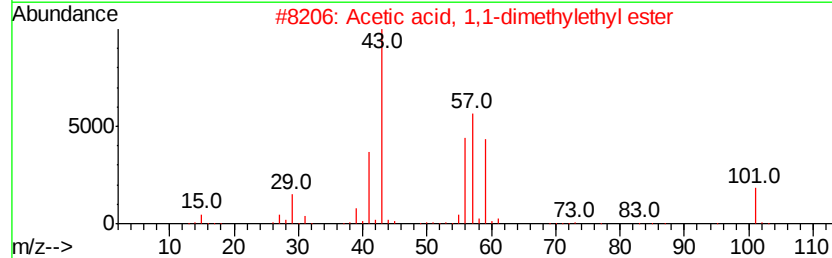
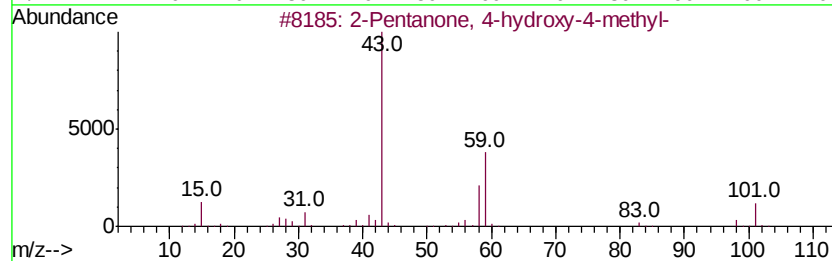
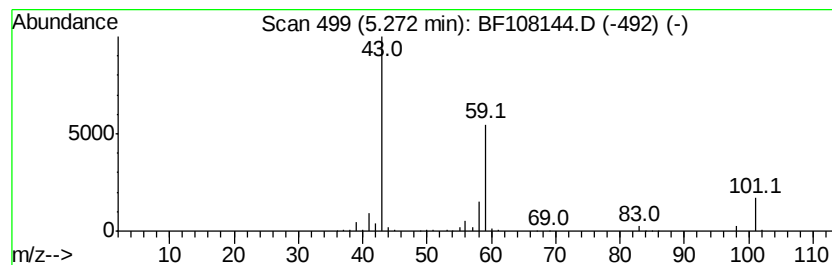
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.27	16.46 ng	828870	1,4-Dichlorobenzene-d4	7.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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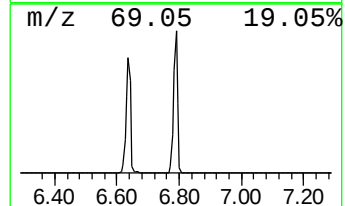
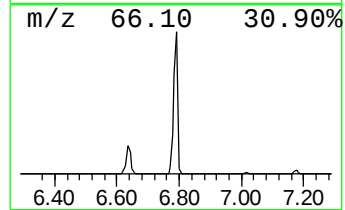
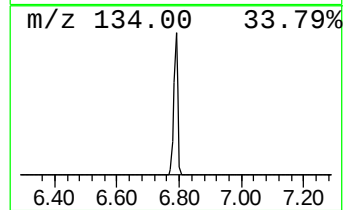
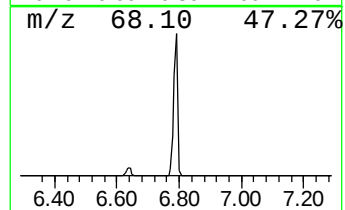
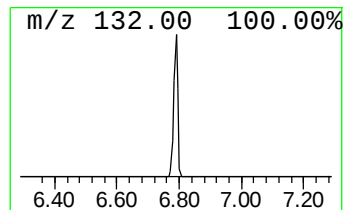
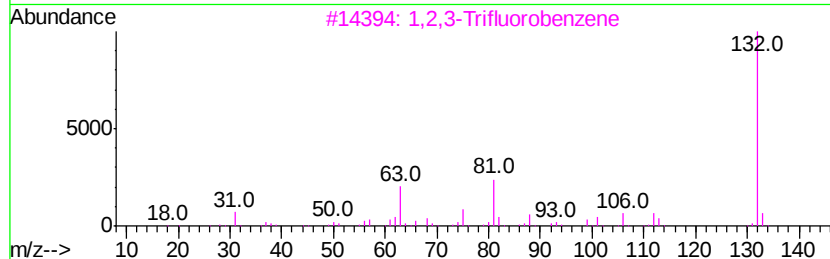
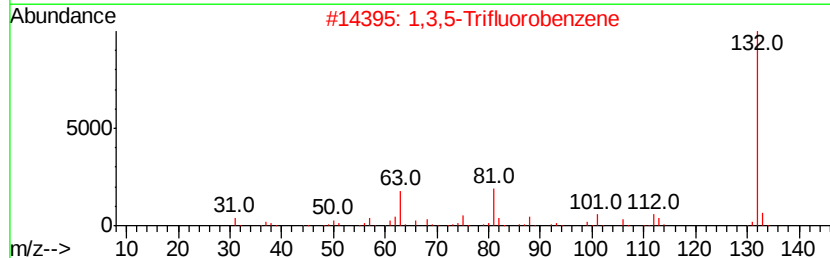
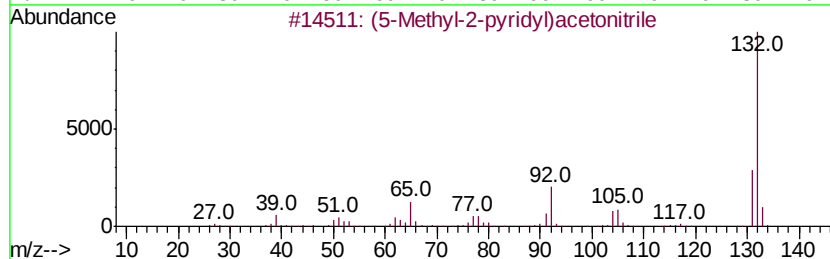
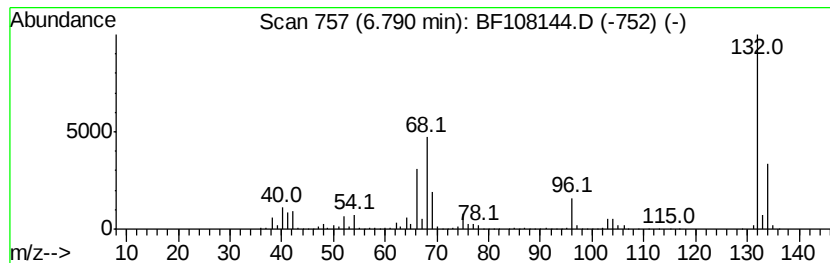
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.79 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.79	77.88 ng	3922510	1,4-Dichlorobenzene-d4	7.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
2		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
3		1,2,3-Trifluorobenzene	132	C6H3F3	001489-53-8	9
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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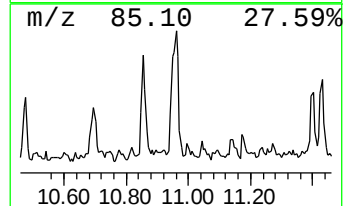
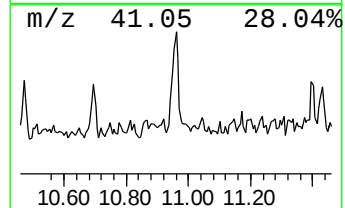
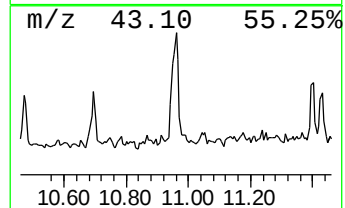
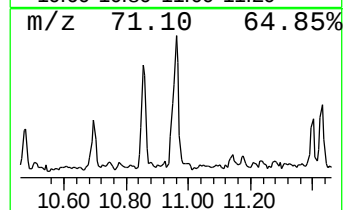
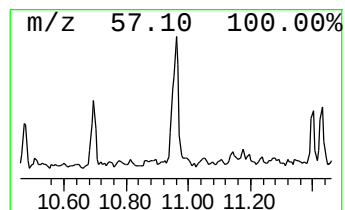
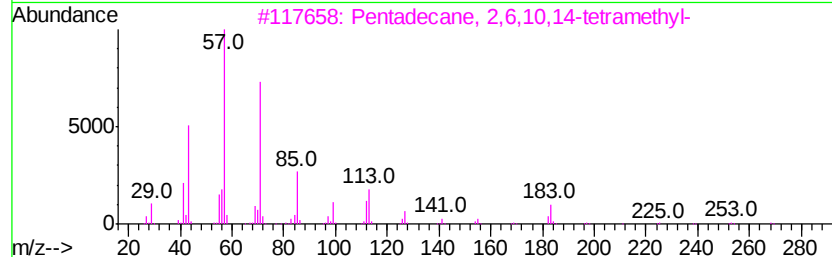
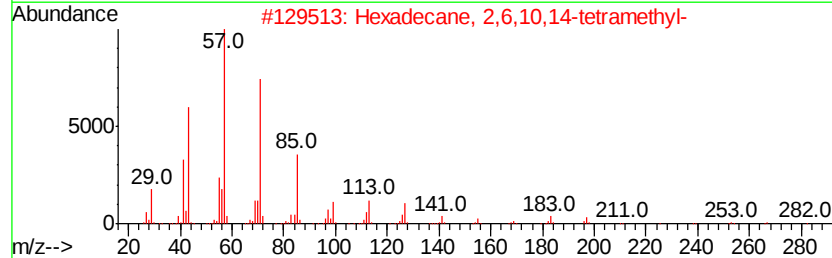
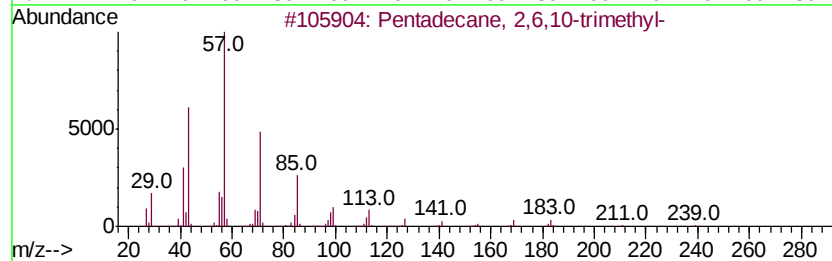
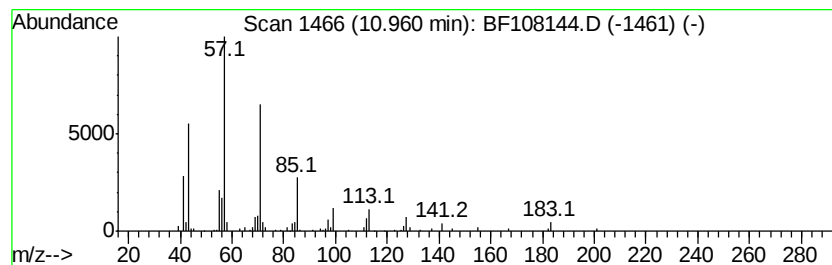
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Pentadecane, 2,6,10-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.96	2.88 ng	155772	Phenanthrene-d10	11.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	90
2		Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	86
3		Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	72
4		Tetradecane, 4-ethyl-	226	C16H34	055045-14-2	64
5		Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	59



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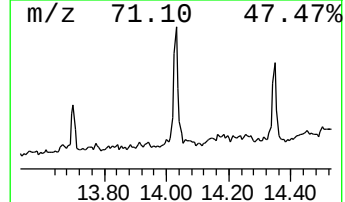
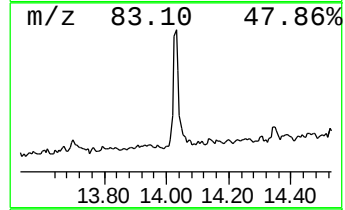
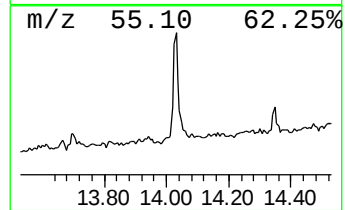
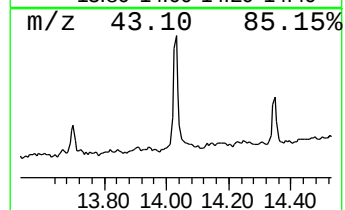
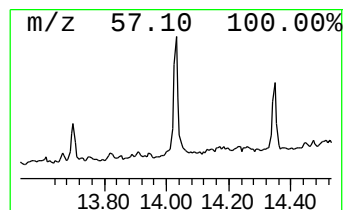
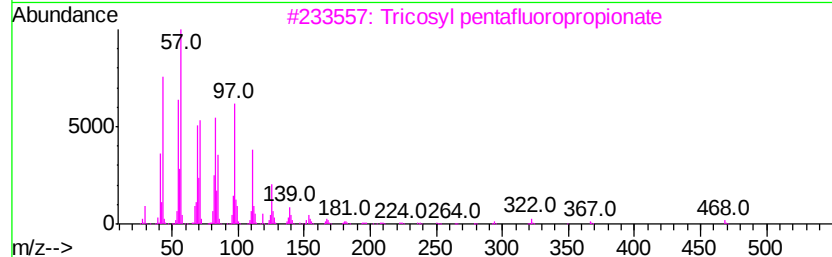
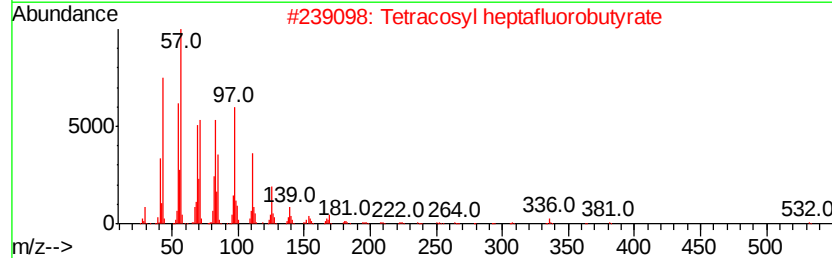
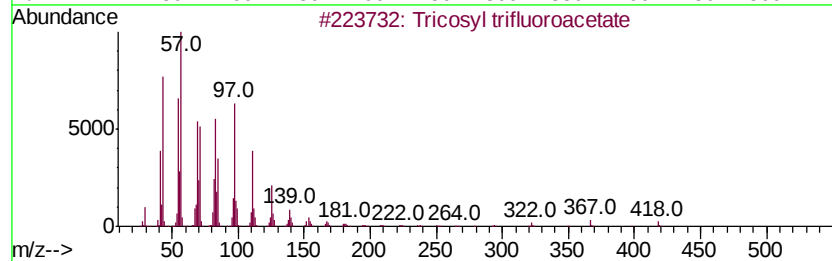
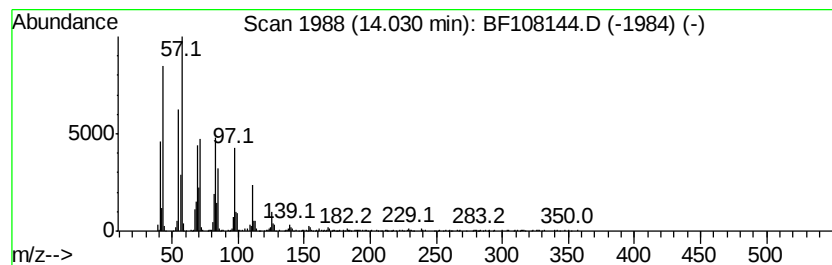
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Tricosyl trifluoroacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.03	8.43 ng	480037	Chrysene-d12	14.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
2		Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	91
3		Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	91
4		Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	91
5		Octacosyl heptafluorobutyrate	606	C32H57F7O2	1000351-83-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081418\
Data File : BF108144.D
Acq On : 14 Aug 2018 15:00
Operator : JU/SJ
Sample : J4447-36
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1-10

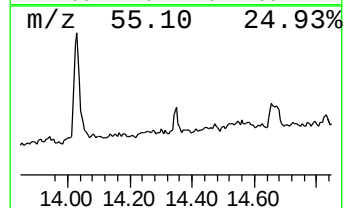
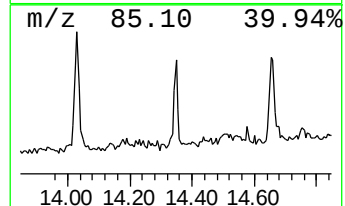
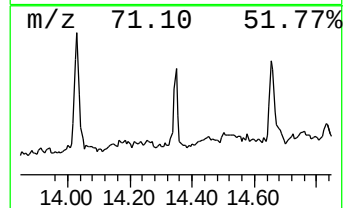
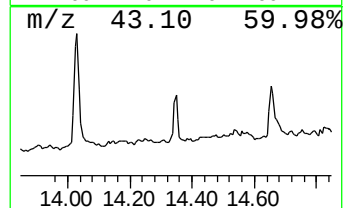
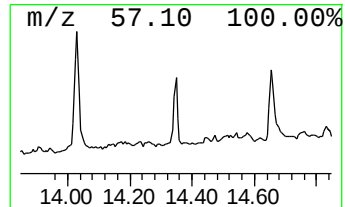
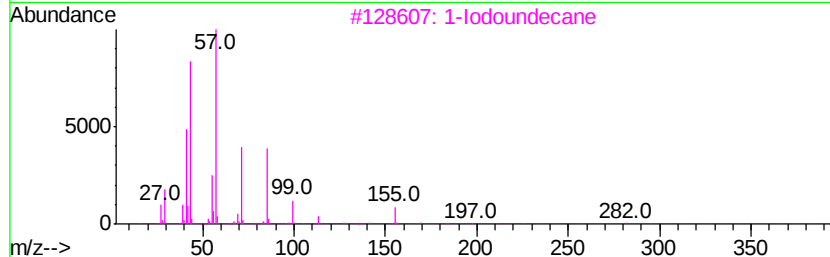
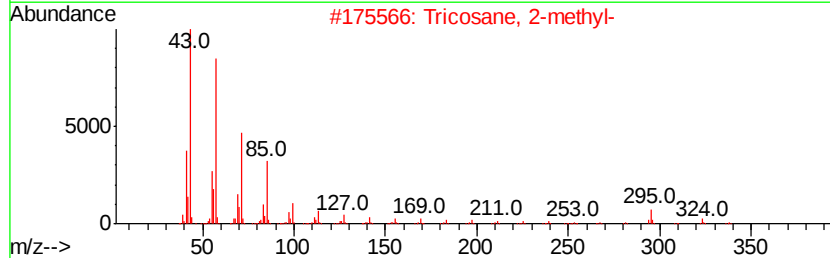
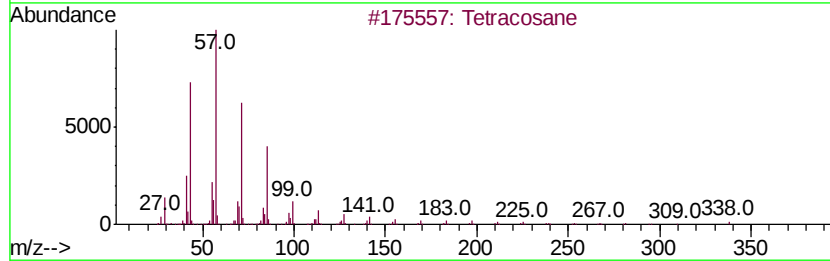
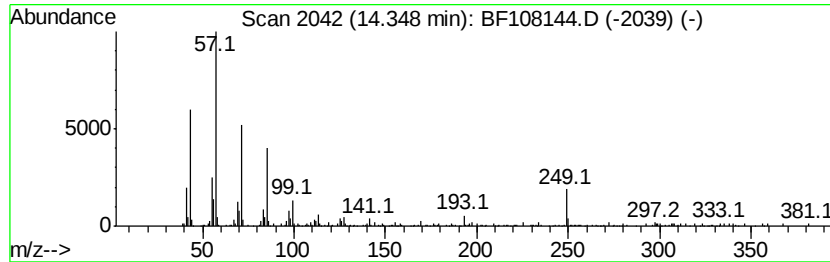
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetracosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.35	2.76 ng	157215	Chrysene-d12	14.22

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetracosane	338	C24H50	000646-31-1	94
2		Tricosane, 2-methyl-	338	C24H50	001928-30-9	89
3		1-Iodoundecane	282	C11H23I	004282-44-4	76
4		Octacosane	394	C28H58	000630-02-4	76
5		Hexacosane	366	C26H54	000630-01-3	70



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081418\
Data File : BF108144.D
Acq On : 14 Aug 2018 15:00
Operator : JU/SJ
Sample : J4447-36
Misc :
ALS Vial : 11 Sample Multiplier: 1

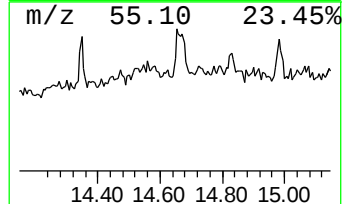
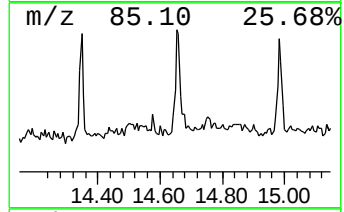
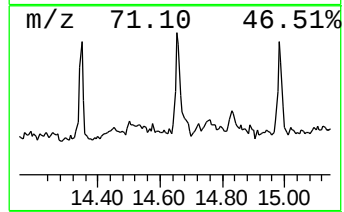
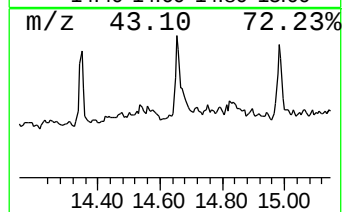
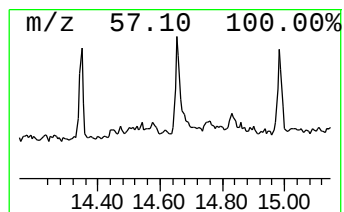
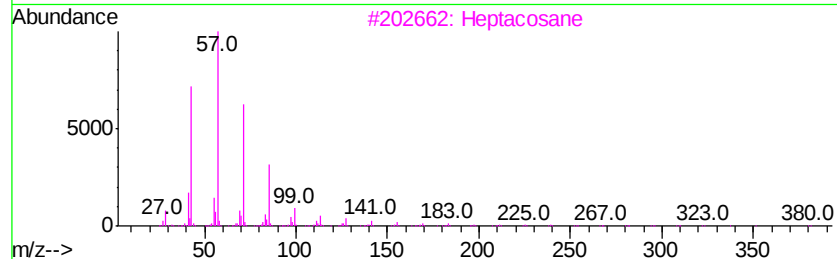
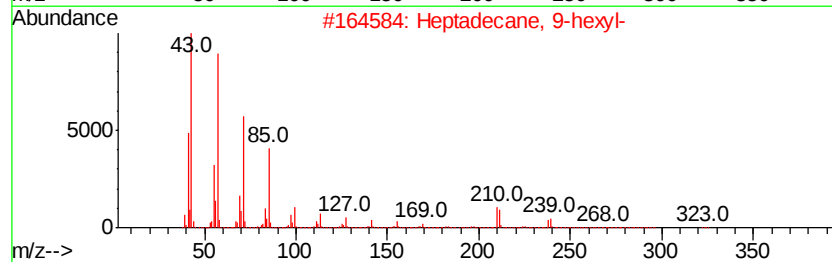
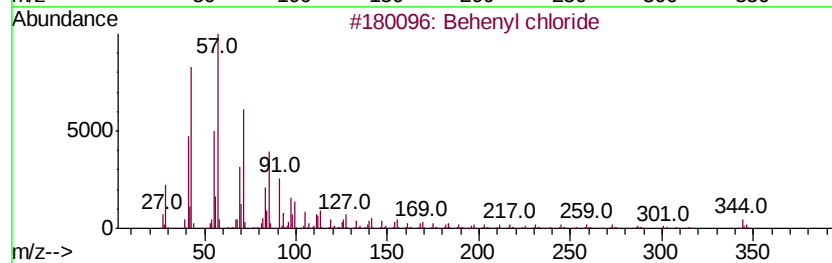
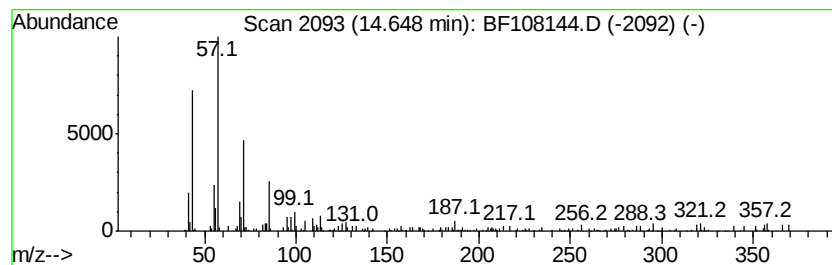
Instrument :
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ClientSampleId :
SP-1-10

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 9 Behenyl chloride Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.65	4.14 ng	235750	Chrysene-d12		14.22
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenyl chloride	344	C22H45Cl	042217-03-8	87
2	Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	87
3	Heptacosane	380	C27H56	000593-49-7	83
4	Tetracosane	338	C24H50	000646-31-1	83
5	Hentriacontane	437	C31H64	000630-04-6	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081418\
Data File : BF108144.D
Acq On : 14 Aug 2018 15:00
Operator : JU/SJ
Sample : J4447-36
Misc :
ALS Vial : 11 Sample Multiplier: 1

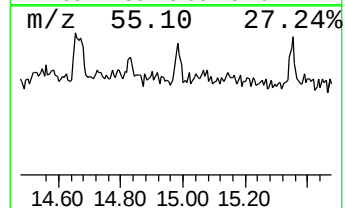
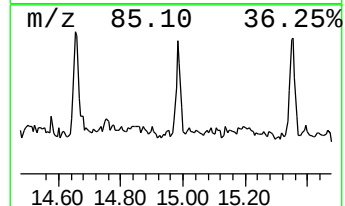
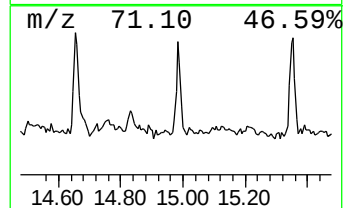
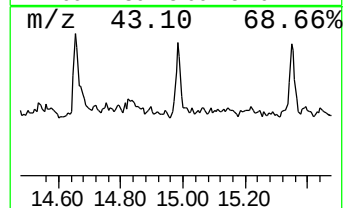
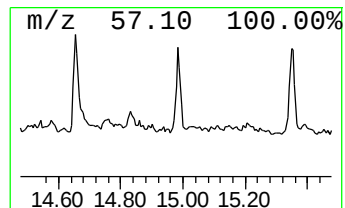
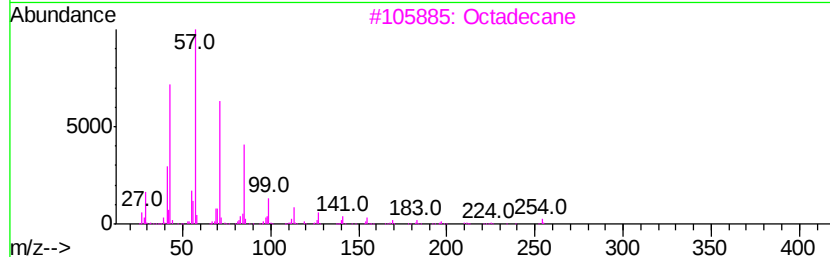
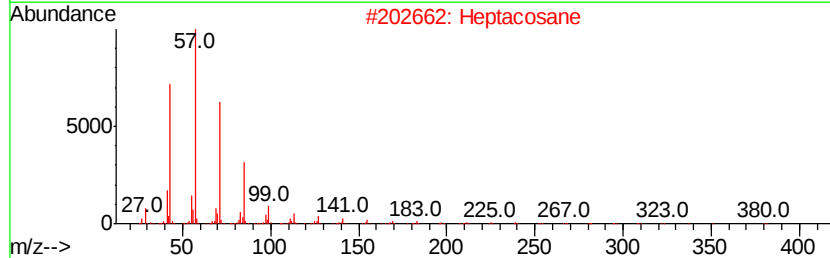
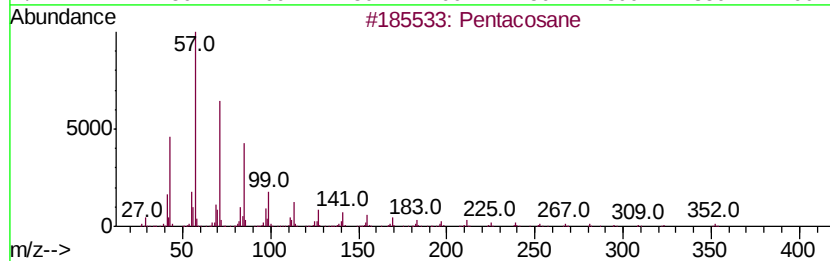
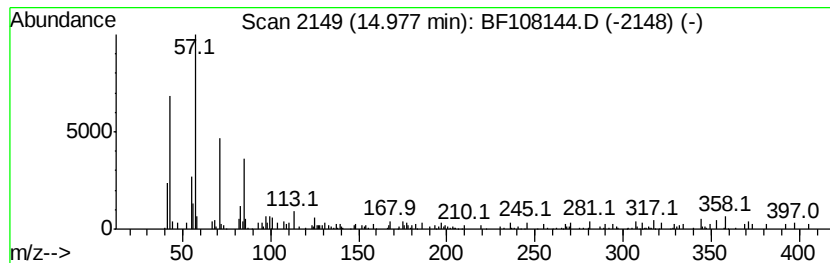
Instrument :
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ClientSampleId :
SP-1-10

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 10 Pentacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	2.02 ng	114916	Chrysene-d12	14.22
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Pentacosane		352 C25H52	000629-99-2 91
2	Heptacosane		380 C27H56	000593-49-7 83
3	Octadecane		254 C18H38	000593-45-3 80
4	Eicosane		282 C20H42	000112-95-8 80
5	Hexadecane		226 C16H34	000544-76-3 80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081418\
Data File : BF108144.D
Acq On : 14 Aug 2018 15:00
Operator : JU/SJ
Sample : J4447-36
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1-10

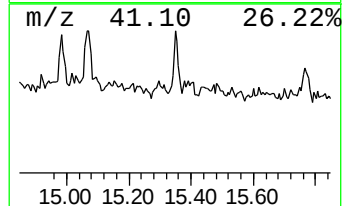
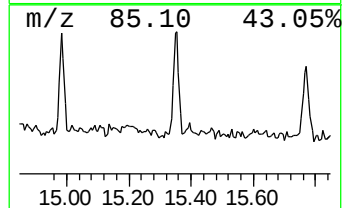
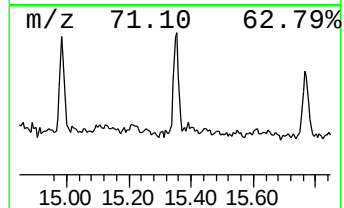
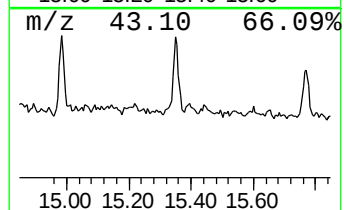
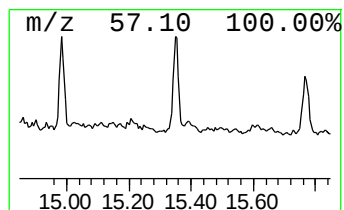
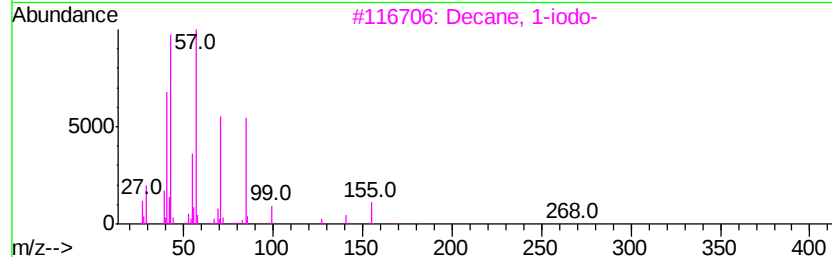
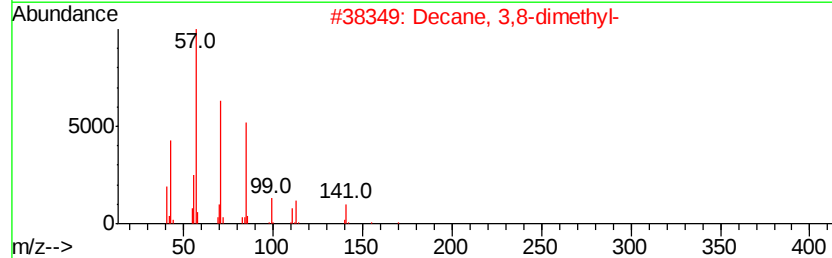
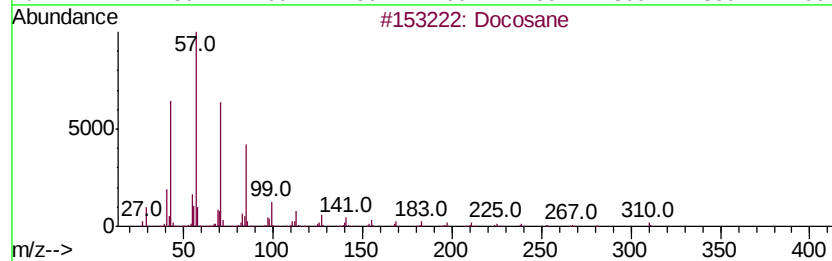
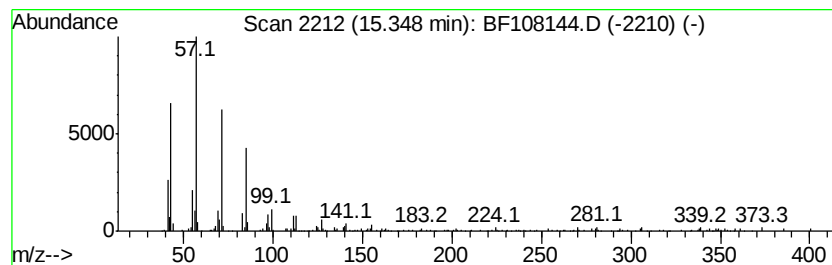
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Docosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.35	3.57 ng	145714	Perylene-d12	15.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Docosane	310	C22H46	000629-97-0	91
2		Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	87
3		Decane, 1-iodo-	268	C10H21I	002050-77-3	83
4		Nonadecane	268	C19H40	000629-92-5	83
5		Heptacosane	380	C27H56	000593-49-7	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081418\
Data File : BF108144.D
Acq On : 14 Aug 2018 15:00
Operator : JU/SJ
Sample : J4447-36
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1-10

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
Butane, 2-methoxy...	2.38	12.4	ng	624673	1	7.02	1007270	20.0
2-Pentanone, 4-hy...	5.27	16.5	ng	828870	1	7.02	1007270	20.0
unknown6.79	6.79	77.9	ng	3922510	1	7.02	1007270	20.0
Pentadecane, 2,6,...	10.96	2.9	ng	155772	4	11.56	1081880	20.0
Tricosyl trifluor...	14.03	8.4	ng	480037	5	14.22	1138770	20.0
Tetracosane	14.35	2.8	ng	157215	5	14.22	1138770	20.0
Behenyl chloride	14.65	4.1	ng	235750	5	14.22	1138770	20.0
Pentacosane	14.98	2.0	ng	114916	5	14.22	1138770	20.0
Docosane	15.35	3.6	ng	145714	6	15.78	816734	20.0