

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091318\
 Data File : BF108971.D
 Acq On : 13 Sep 2018 18:22
 Operator : JU/SJ
 Sample : J4873-03
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NF-CON-2

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-BF090518.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	4.278	325	330	336	rBV	214199	263745	7.12%	0.829%
2	4.919	434	439	453	rVB	559093	690183	18.63%	2.169%
3	5.337	505	510	514	rBV	2469666	2519571	68.02%	7.918%
4	6.360	679	684	687	rBV	2793345	3011044	81.29%	9.463%
5	6.495	703	707	710	rBV	3051319	2813638	75.96%	8.843%
6	6.731	743	747	750	rBV	1017639	892871	24.11%	2.806%
7	6.884	769	773	777	rBV	2781797	2543068	68.66%	7.992%
8	7.289	837	842	845	rBV	2159089	2039905	55.07%	6.411%
9	8.007	960	964	968	rBV	1302246	1120790	30.26%	3.522%
10	9.089	1143	1148	1151	rBV	4004558	3704016	100.00%	11.641%
11	9.478	1210	1214	1217	rBV	859300	638942	17.25%	2.008%
12	9.760	1258	1262	1266	rBV	1496040	1243776	33.58%	3.909%
13	10.178	1327	1333	1335	rBV	34844	39016	1.05%	0.123%
14	10.542	1391	1395	1398	rBV	1771467	1499704	40.49%	4.713%
15	10.678	1414	1418	1420	rBV	95601	94654	2.56%	0.297%
16	11.125	1487	1494	1496	rBV2	95820	82253	2.22%	0.259%
17	11.154	1496	1499	1504	rVB	45528	44166	1.19%	0.139%
18	11.236	1509	1513	1516	rBV	1451721	1166012	31.48%	3.665%
19	11.548	1563	1566	1569	rBV	109618	84986	2.29%	0.267%
20	11.772	1600	1604	1608	rBV4	56396	66843	1.80%	0.210%
21	11.954	1632	1635	1640	rVB	100539	78727	2.13%	0.247%
22	12.342	1698	1701	1704	rVB	79937	62242	1.68%	0.196%
23	12.713	1761	1764	1766	rBV	65332	51768	1.40%	0.163%
24	12.819	1778	1782	1786	rBV	3119589	3008170	81.21%	9.454%
25	13.066	1821	1824	1827	rVB	49608	42242	1.14%	0.133%
26	13.407	1879	1882	1885	rBV	52560	40438	1.09%	0.127%
27	13.736	1934	1938	1952	rBV4	92364	191951	5.18%	0.603%
28	13.860	1955	1959	1963	rVV	1134571	1016597	27.45%	3.195%
29	14.048	1988	1991	1994	rBV	73322	63112	1.70%	0.198%
30	14.354	2040	2043	2046	rBV	117191	102669	2.77%	0.323%
31	14.648	2090	2093	2098	rVV	152027	146522	3.96%	0.460%
32	14.718	2102	2105	2109	rVB	98106	95185	2.57%	0.299%
33	14.965	2143	2147	2152	rBV	185467	217350	5.87%	0.683%
34	15.271	2194	2199	2203	rBV	946999	1085416	29.30%	3.411%

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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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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.324	2203	2208	2215	rVV	244945	325891	8.80%	1.024%
36	15.730	2272	2277	2285	rBV	214574	333964	9.02%	1.050%
37	16.201	2352	2357	2365	rVB2	126058	228116	6.16%	0.717%
38	16.754	2445	2451	2456	rVB2	50902	102528	2.77%	0.322%
39	17.395	2556	2560	2570	rVB8	27018	67023	1.81%	0.211%

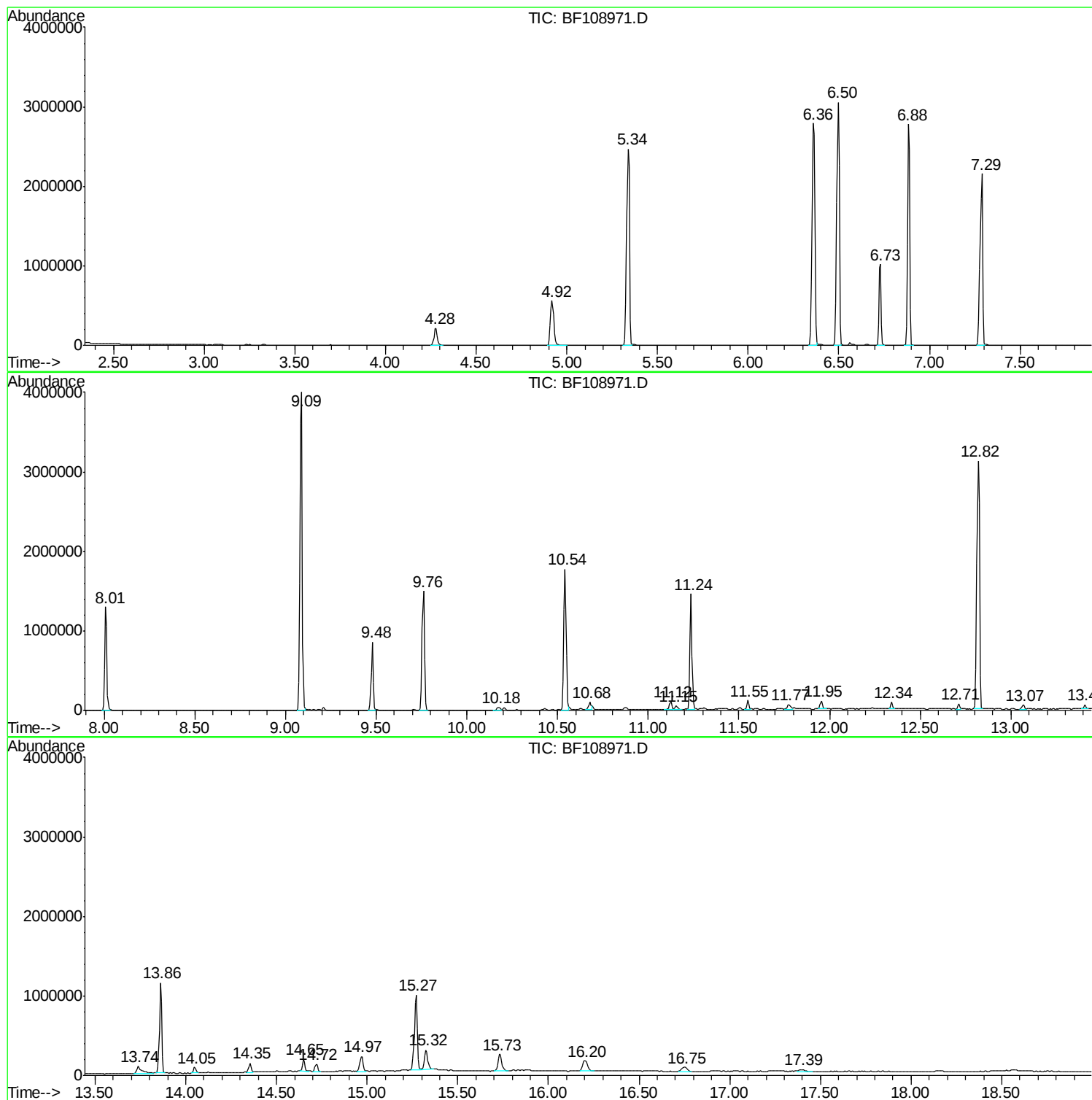
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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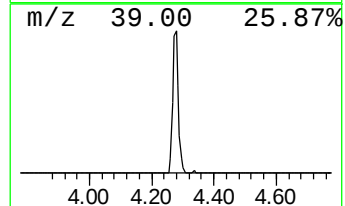
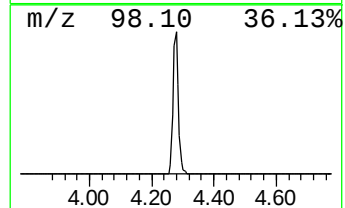
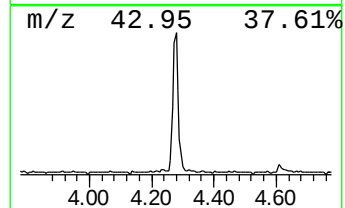
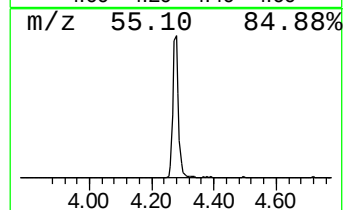
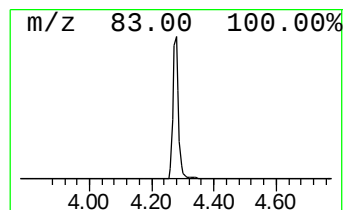
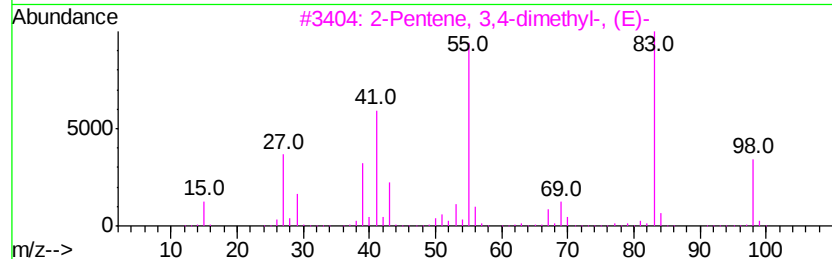
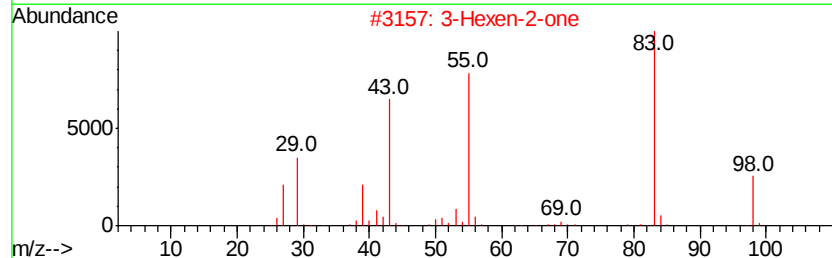
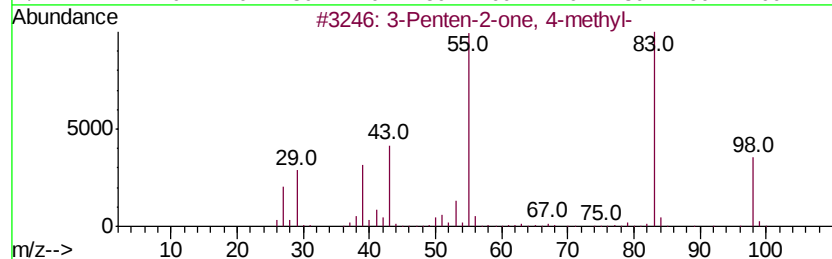
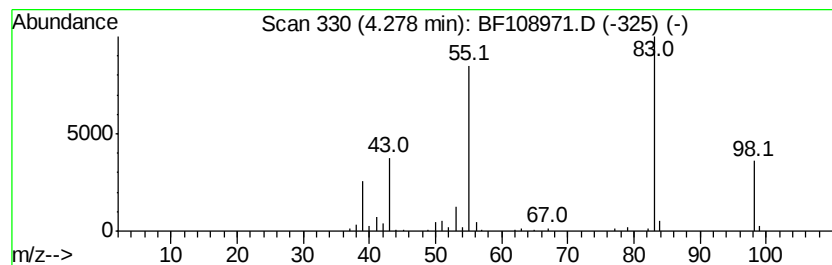
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.28	5.91 ng	263745	1,4-Dichlorobenzene-d4	6.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80



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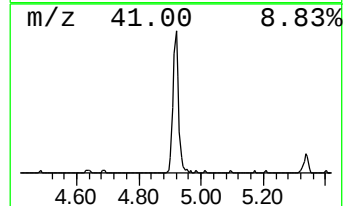
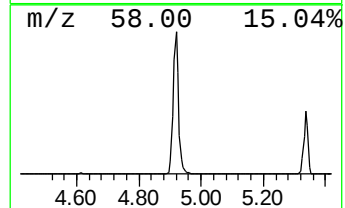
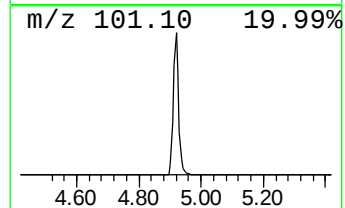
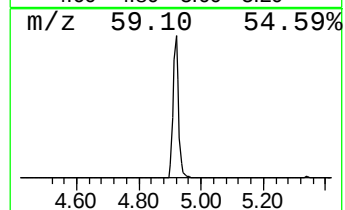
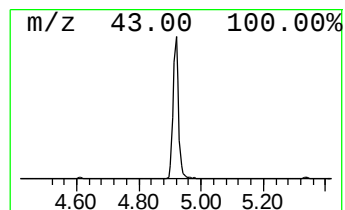
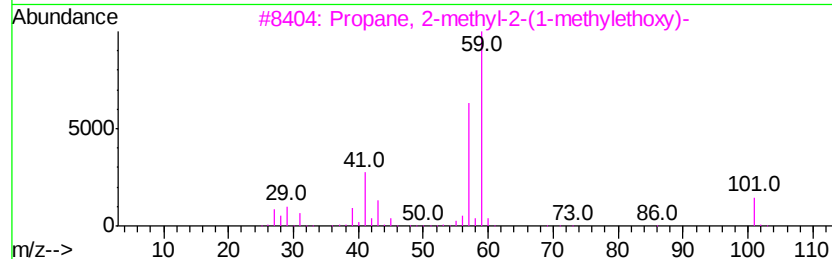
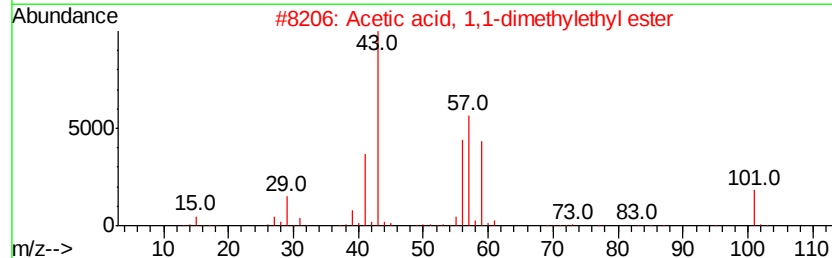
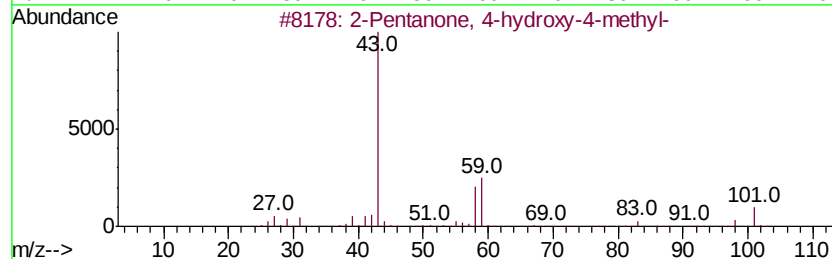
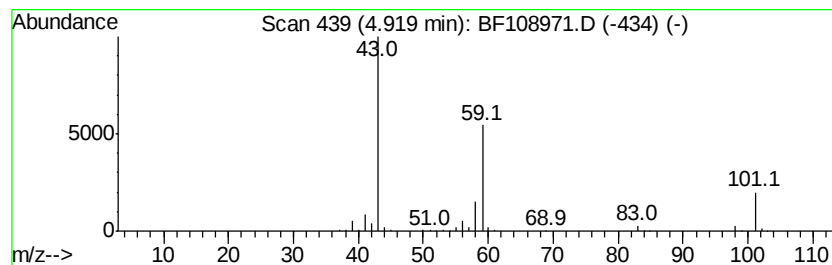
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	15.46 ng	690183	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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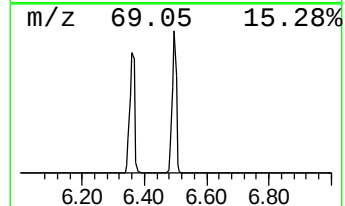
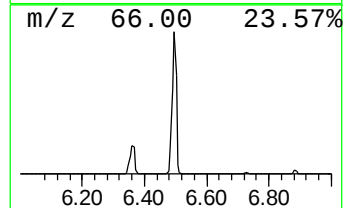
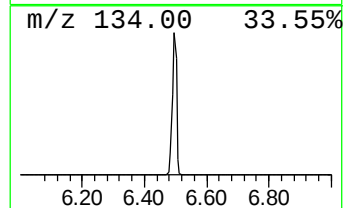
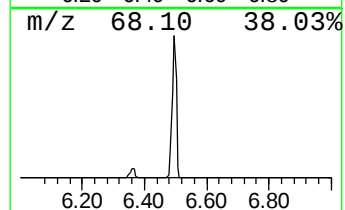
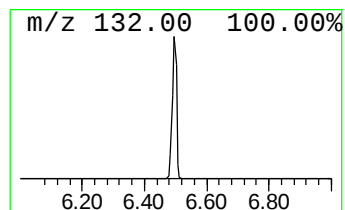
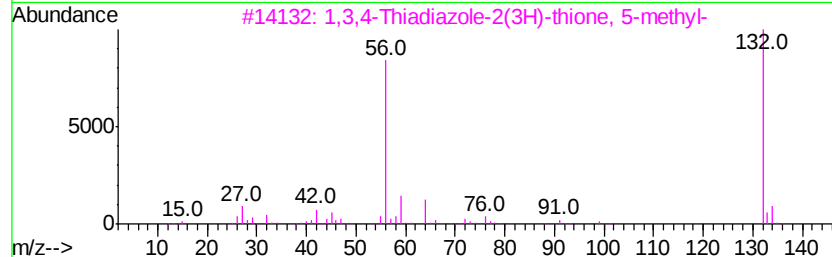
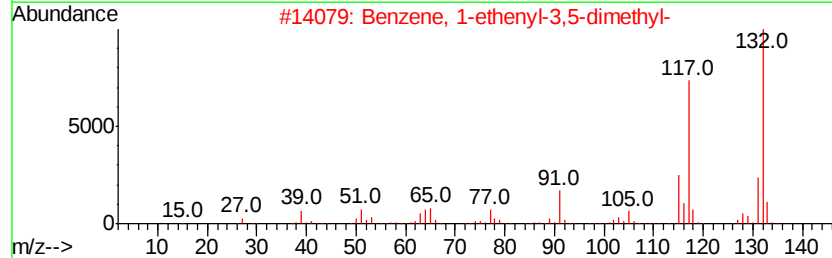
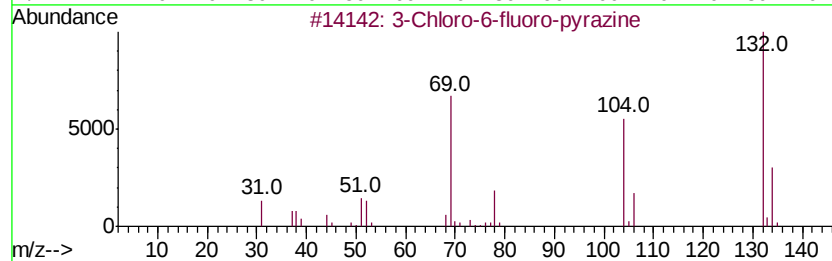
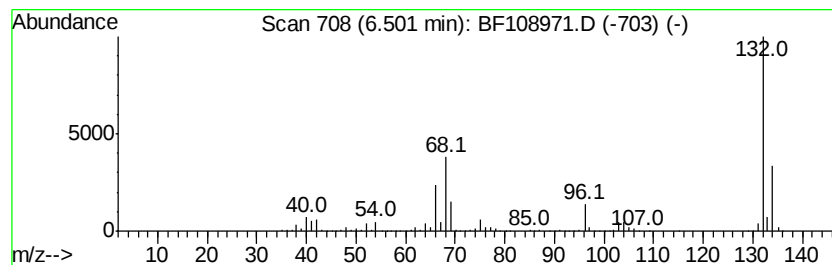
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	63.02 ng	2813640	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
3		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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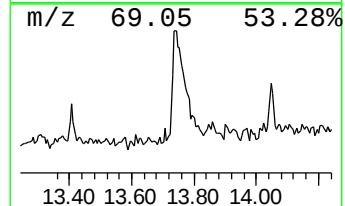
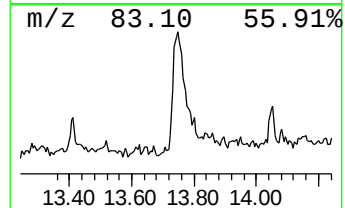
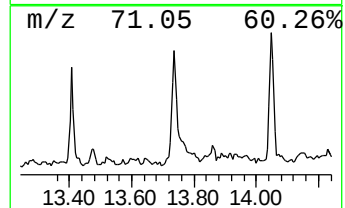
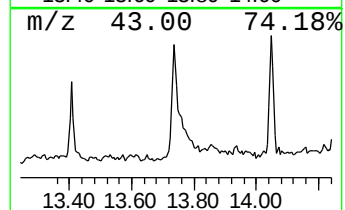
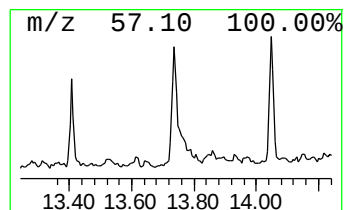
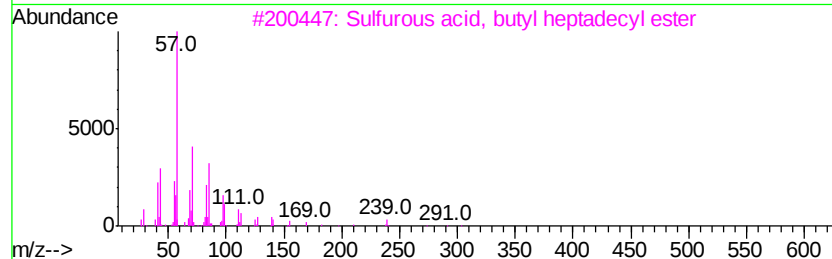
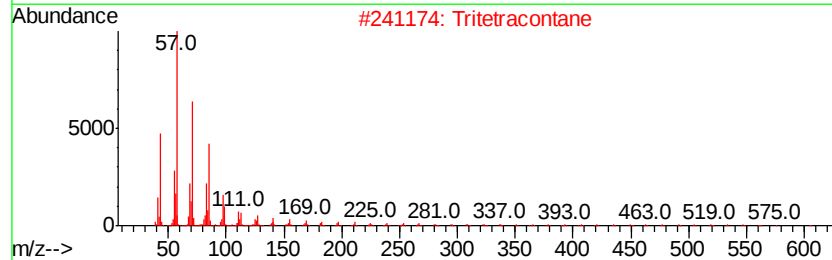
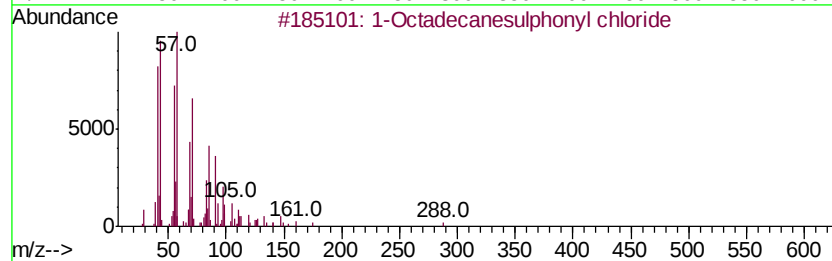
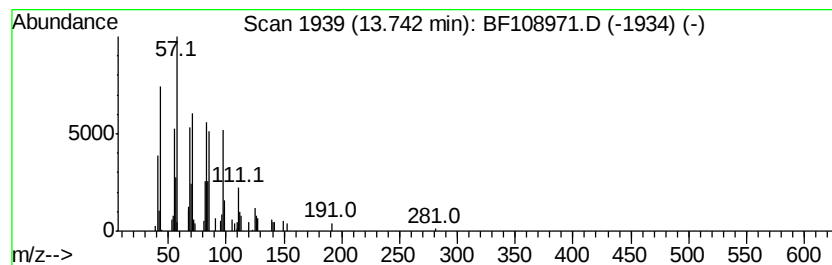
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Octadecanesulphonyl chloride Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	3.78 ng	191951	Chrysene-d12	13.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	91
2		Tritetracontane	605	C43H88	007098-21-7	87
3		Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	74
4		Tetradecane	198	C14H30	000629-59-4	68
5		Hexadecane	226	C16H34	000544-76-3	64



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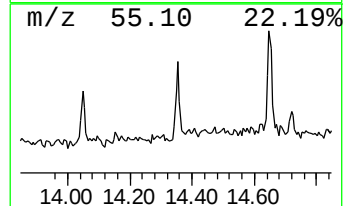
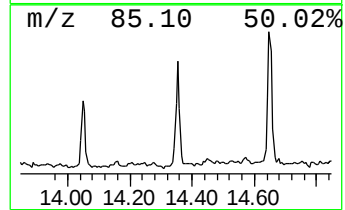
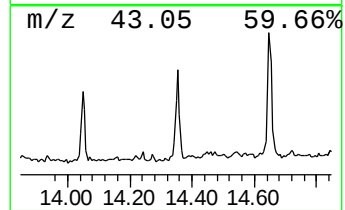
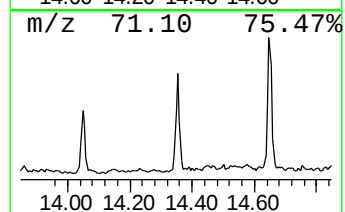
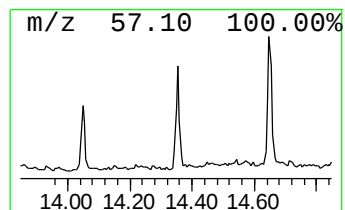
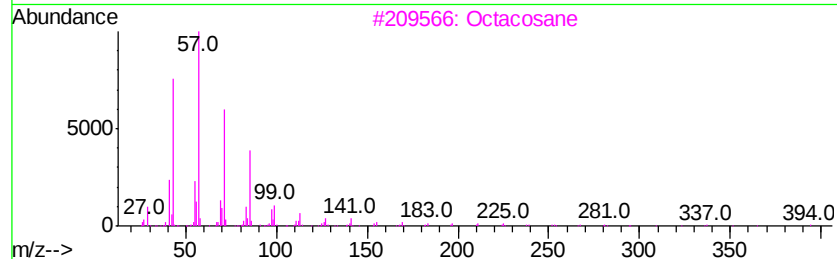
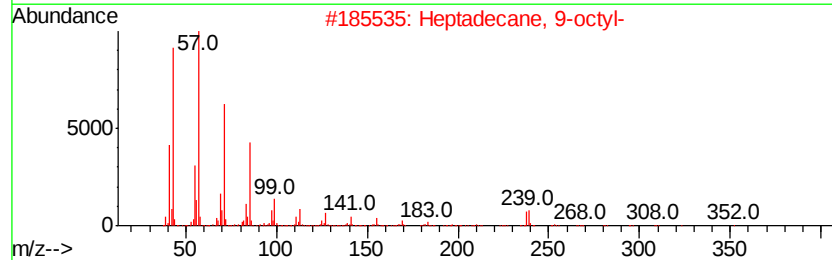
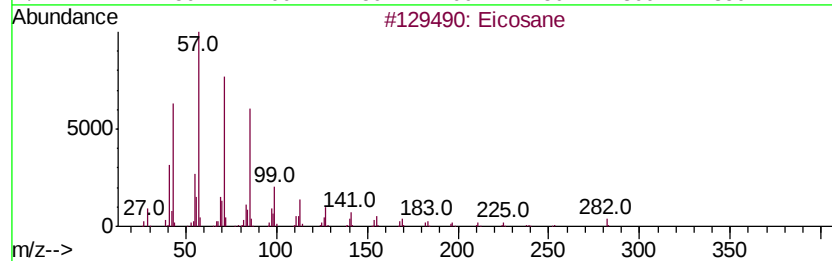
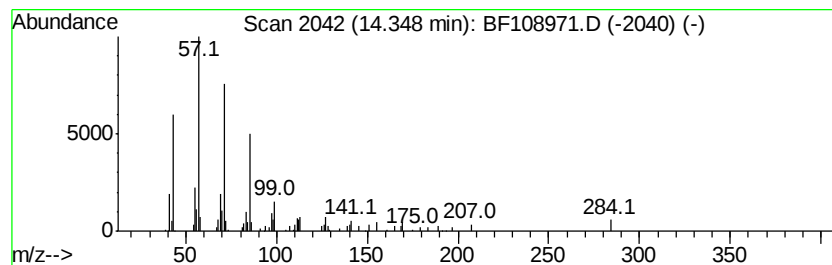
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Eicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.35	2.02 ng	102669	Chrysene-d12	13.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	94
2	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91
3	Octacosane		394	C28H58	000630-02-4	91
4	Heneicosane		296	C21H44	000629-94-7	90
5	Octadecane		254	C18H38	000593-45-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091318\
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Acq On : 13 Sep 2018 18:22
Operator : JU/SJ
Sample : J4873-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NF-CON-2

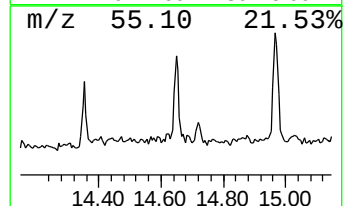
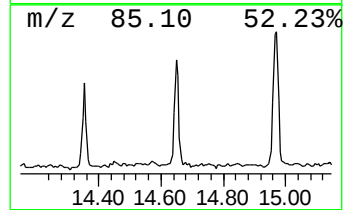
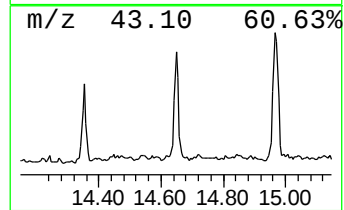
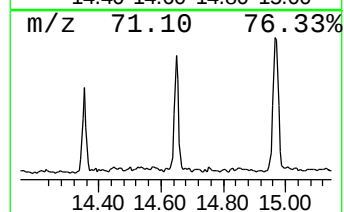
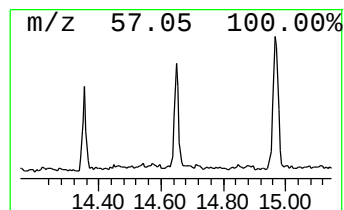
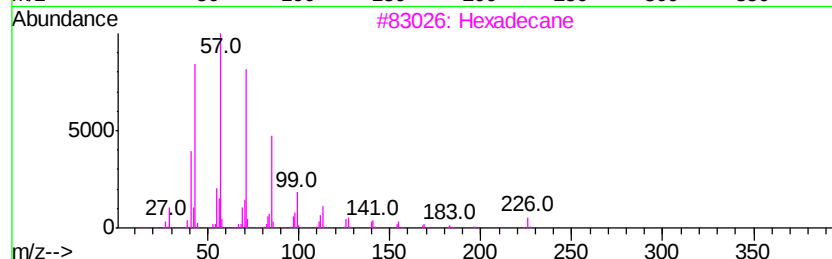
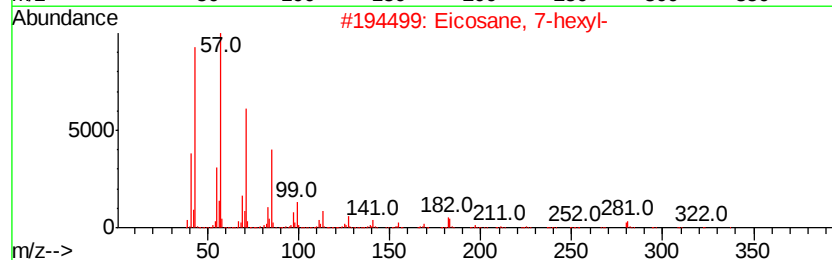
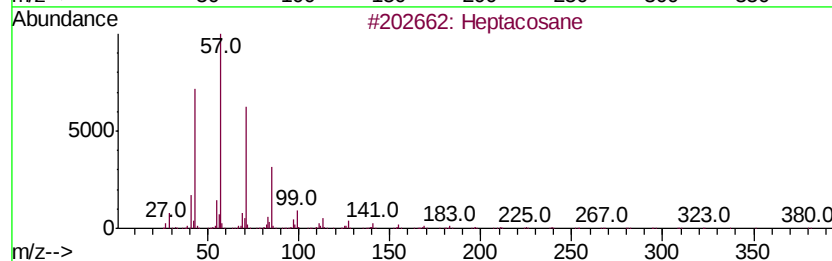
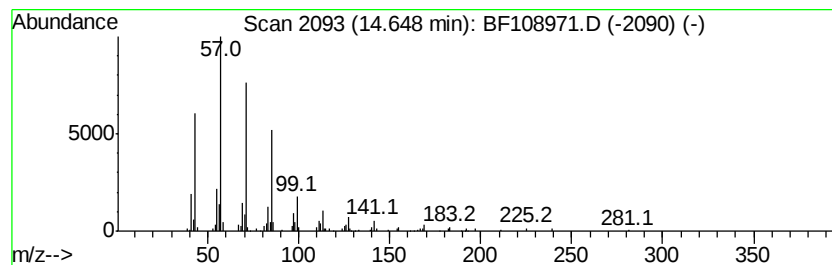
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.65	2.70 ng	146522	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	91
2		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
3		Hexadecane	226	C16H34	000544-76-3	90
4		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	90
5		Heneicosane	296	C21H44	000629-94-7	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091318\
Data File : BF108971.D
Acq On : 13 Sep 2018 18:22
Operator : JU/SJ
Sample : J4873-03
Misc :
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Instrument :
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ClientSampleId :
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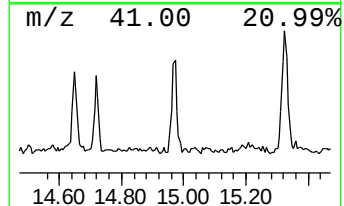
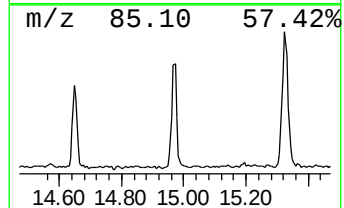
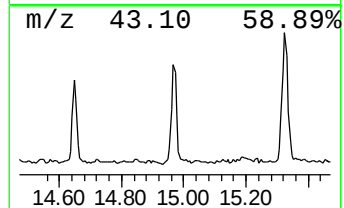
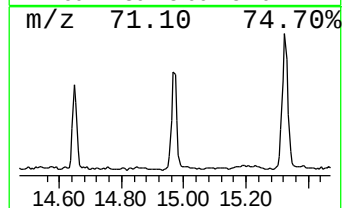
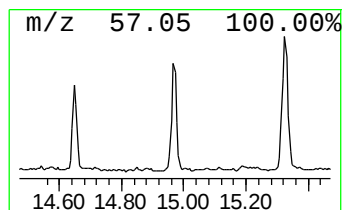
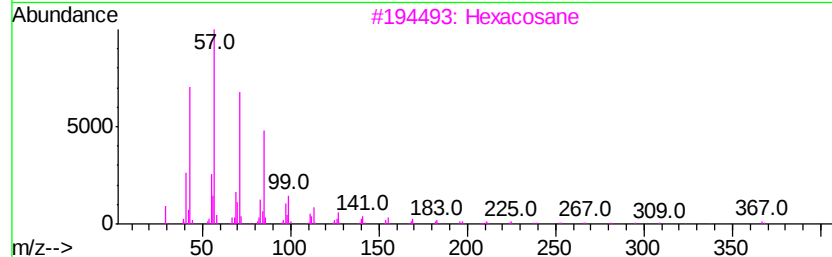
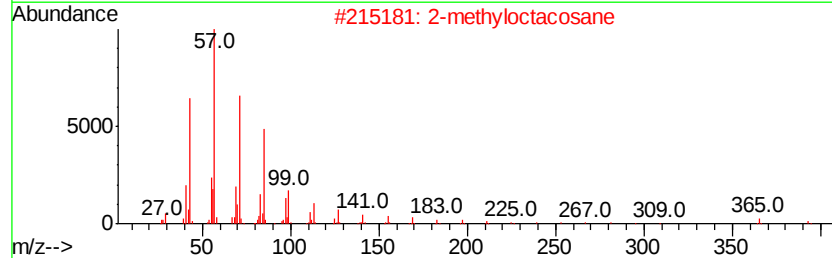
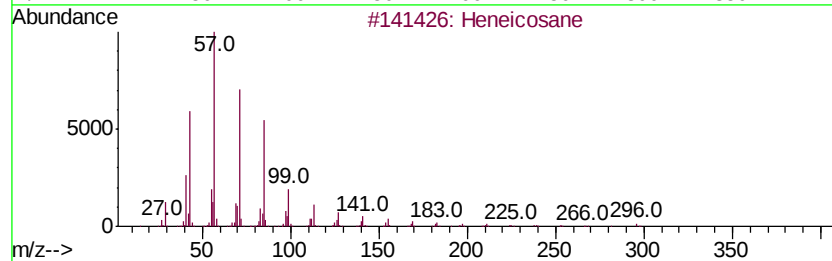
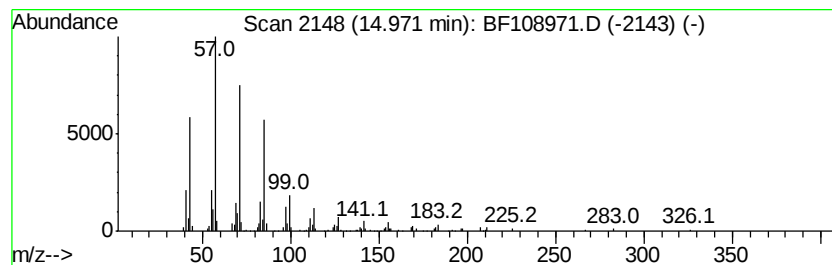
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.97	4.00 ng	217350	Perylene-d12	15.27

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	2-methyloctacosane		408	C29H60	1000376-72-8	91
3	Hexacosane		366	C26H54	000630-01-3	90
4	Octacosane		394	C28H58	000630-02-4	90
5	Tetracosane		338	C24H50	000646-31-1	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091318\
 Data File : BF108971.D
 Acq On : 13 Sep 2018 18:22
 Operator : JU/SJ
 Sample : J4873-03
 Misc :
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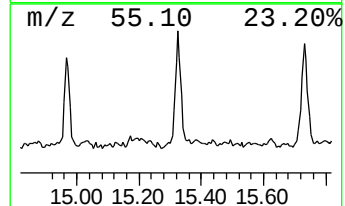
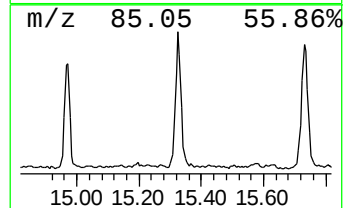
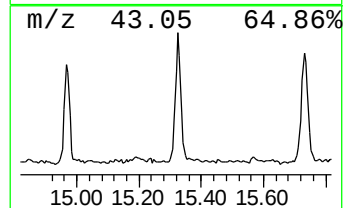
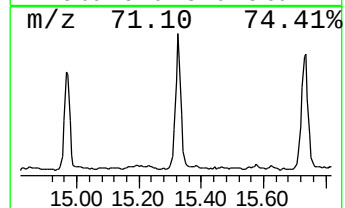
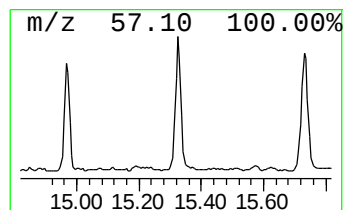
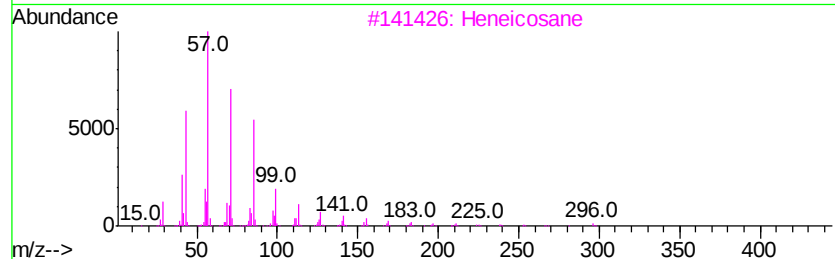
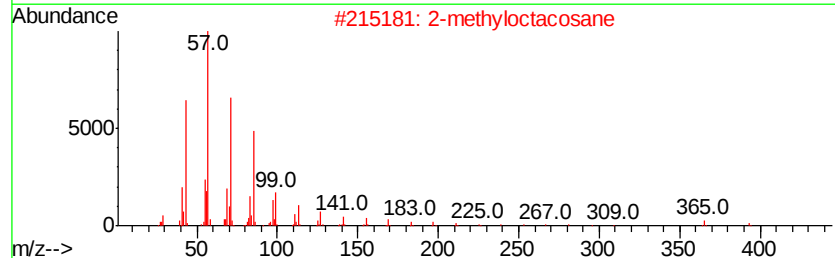
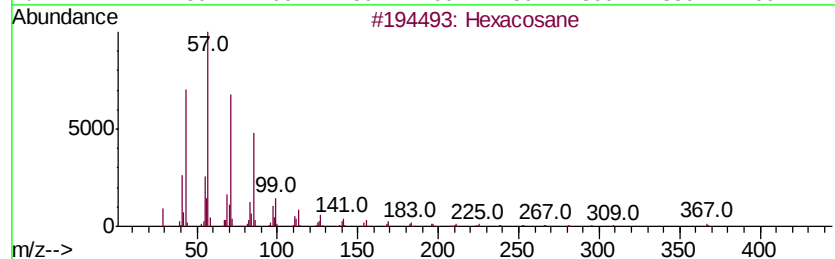
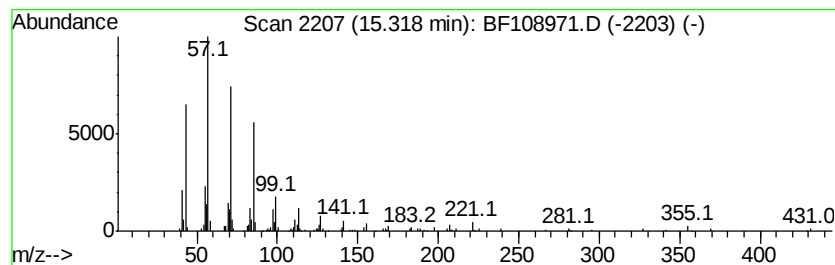
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF090518.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 9 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.32	6.00 ng	325891	Perylene-d12		15.27	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexacosane	366	C26H54	000630-01-3	94
2		2-methyloctacosane	408	C29H60	1000376-72-8	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Tetracosane	338	C24H50	000646-31-1	91
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091318\
Data File : BF108971.D
Acq On : 13 Sep 2018 18:22
Operator : JU/SJ
Sample : J4873-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NF-CON-2

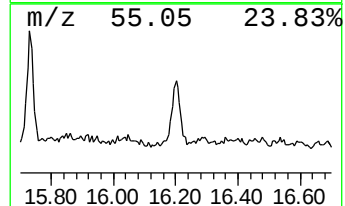
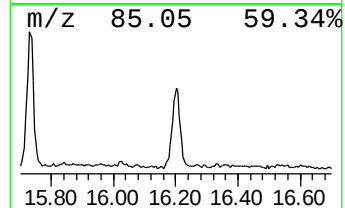
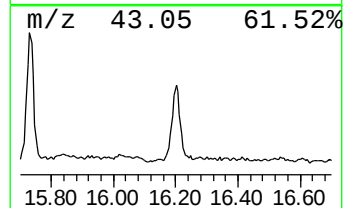
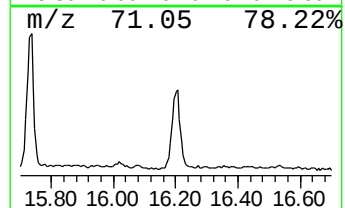
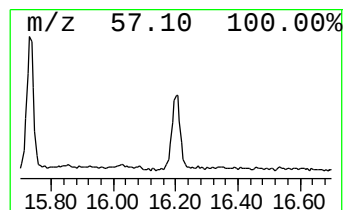
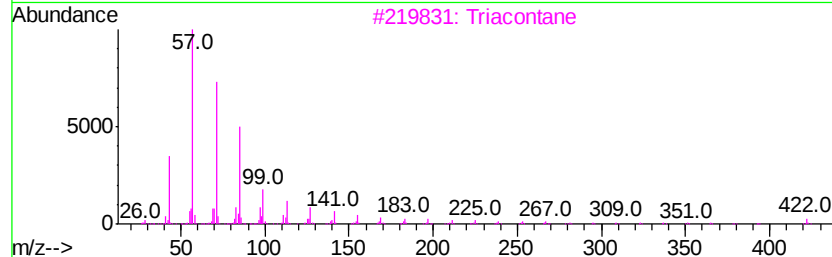
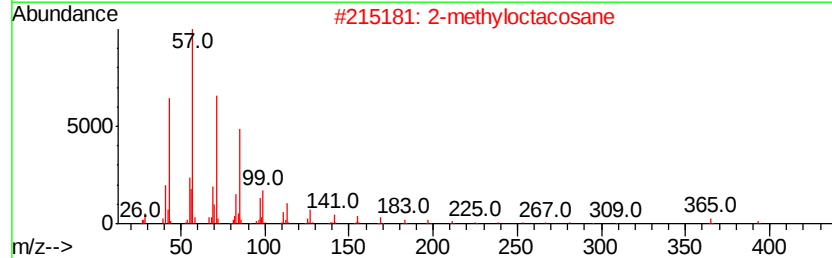
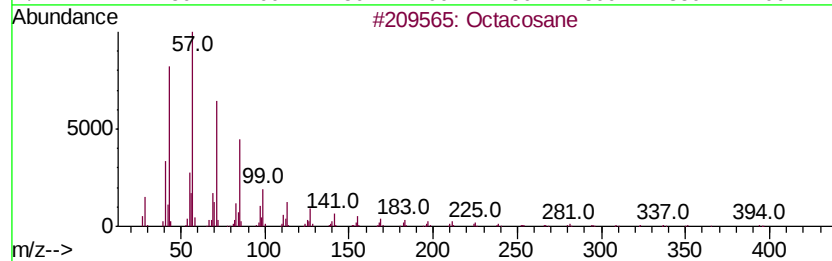
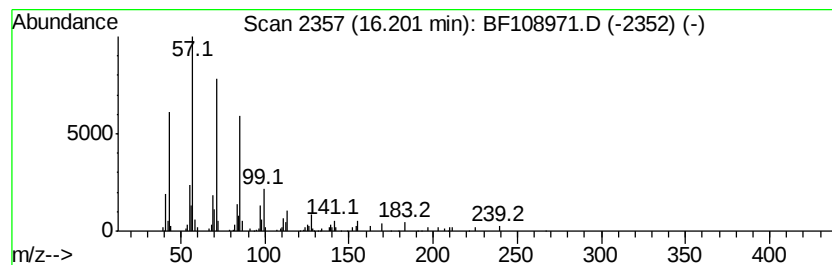
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.20	4.20 ng	228116	Perylene-d12	15.27

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			2-methyloctacosane	408	C29H60	1000376-72-8	91
3			Triacontane	422	C30H62	000638-68-6	91
4			Heneicosane	296	C21H44	000629-94-7	90
5			Hexacosane	366	C26H54	000630-01-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091318\
Data File : BF108971.D
Acq On : 13 Sep 2018 18:22
Operator : JU/SJ
Sample : J4873-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NF-CON-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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...	4.92	15.5	ng	690183	1	6.73	892871	20.0
unknown6.50	6.50	63.0	ng	2813640	1	6.73	892871	20.0
1-Octadecanesulph...	13.74	3.8	ng	191951	5	13.86	1016600	20.0
Eicosane	14.35	2.0	ng	102669	5	13.86	1016600	20.0
Heptacosane	14.65	2.7	ng	146522	6	15.27	1085420	20.0
Heneicosane	14.97	4.0	ng	217350	6	15.27	1085420	20.0
Hexacosane	15.32	6.0	ng	325891	6	15.27	1085420	20.0
Octacosane	16.20	4.2	ng	228116	6	15.27	1085420	20.0