

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102517\
 Data File : BF099844.D
 Acq On : 26 Oct 2017 6:35
 Operator : SJ/JU
 Sample : I6057-03
 Misc :
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 101917-TIDO-F-U-B

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:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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	4.998	492	495	506	rBV	56038	77362	3.56%	0.574%
2	5.410	562	565	581	rBV	424263	537476	24.76%	3.985%
3	6.434	737	739	755	rBV	291871	358211	16.50%	2.656%
4	6.563	758	761	775	rVB	1198679	1052895	48.50%	7.807%
5	6.792	797	800	810	rBV	459478	396615	18.27%	2.941%
6	6.945	823	826	839	rBV	1624009	1482256	68.27%	10.991%
7	7.363	893	897	921	rBV	1212007	1086441	50.04%	8.056%
8	8.075	1015	1018	1037	rBV	647272	549261	25.30%	4.073%
9	9.157	1197	1202	1205	rBV	2438171	2171090	100.00%	16.099%
10	9.551	1266	1269	1277	rBV	92822	77855	3.59%	0.577%
11	9.833	1312	1317	1326	rVB	664888	620622	28.59%	4.602%
12	10.510	1429	1432	1436	rBB	44946	33797	1.56%	0.251%
13	10.633	1449	1453	1465	rBV	806306	783957	36.11%	5.813%
14	11.327	1568	1571	1580	rBV	670882	595352	27.42%	4.415%
15	12.916	1837	1841	1845	rBV	2082971	2105884	97.00%	15.616%
16	13.980	2019	2022	2030	rBV	625127	569740	26.24%	4.225%
17	15.427	2263	2268	2269	rBV	40026	47250	2.18%	0.350%
18	15.451	2269	2272	2286	rVB	398430	508906	23.44%	3.774%
19	15.851	2332	2340	2348	rBV2	50911	80705	3.72%	0.598%
20	16.339	2418	2423	2432	rVB	53796	95011	4.38%	0.705%
21	16.921	2515	2522	2530	rVB2	38928	82907	3.82%	0.615%
22	17.598	2629	2637	2647	rBV3	34304	88862	4.09%	0.659%
23	18.403	2765	2774	2784	rBV3	19583	59785	2.75%	0.443%
24	19.368	2933	2938	2946	rVB5	9539	23617	1.09%	0.175%

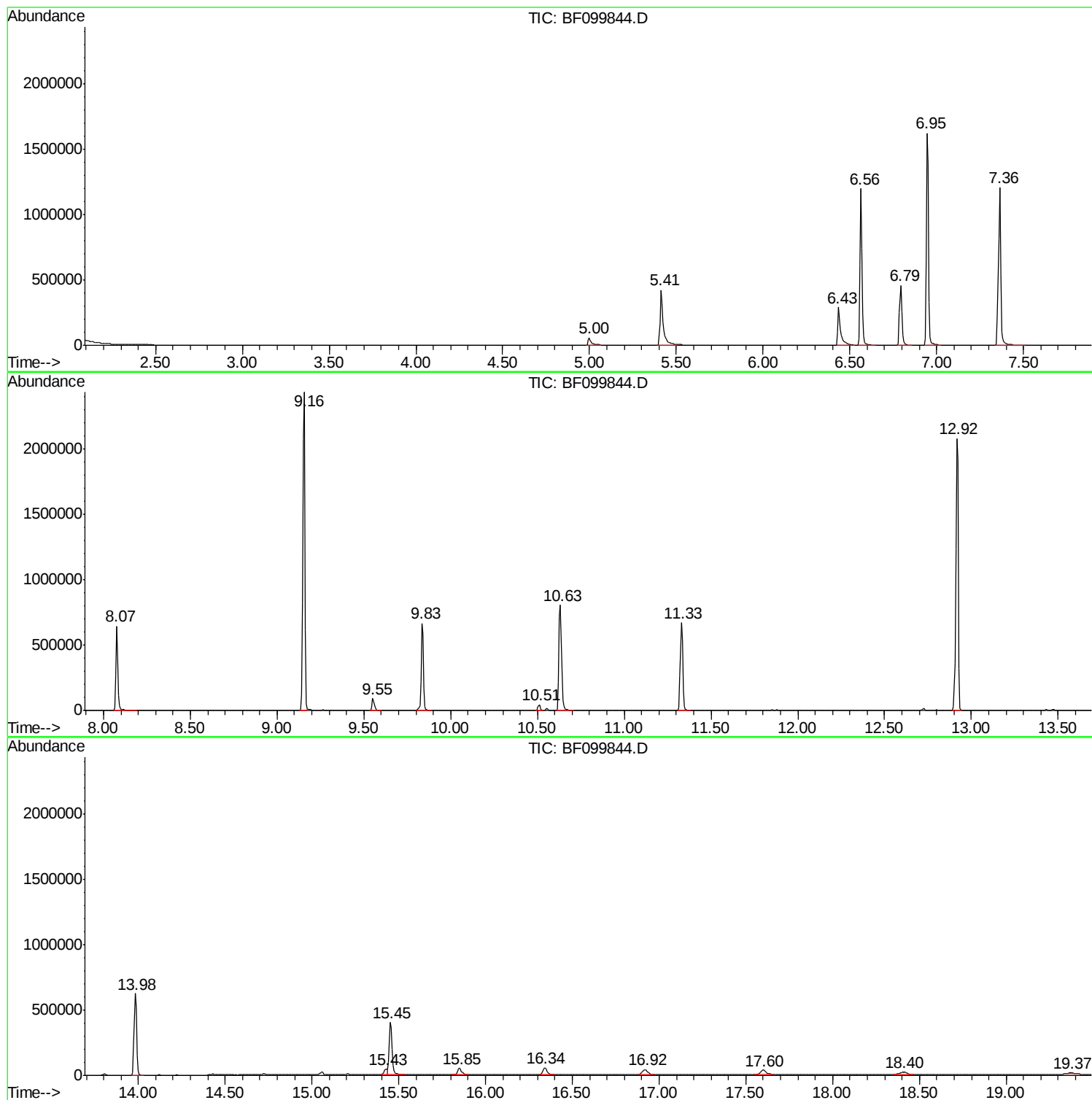
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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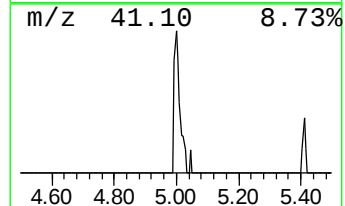
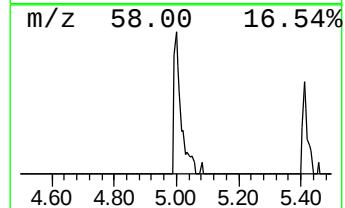
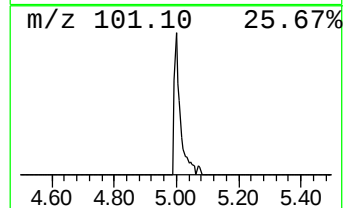
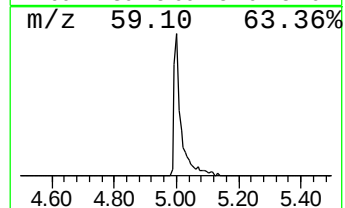
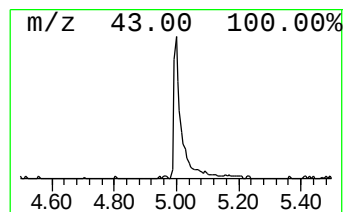
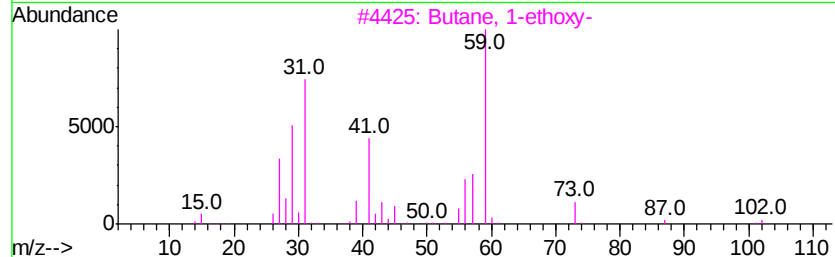
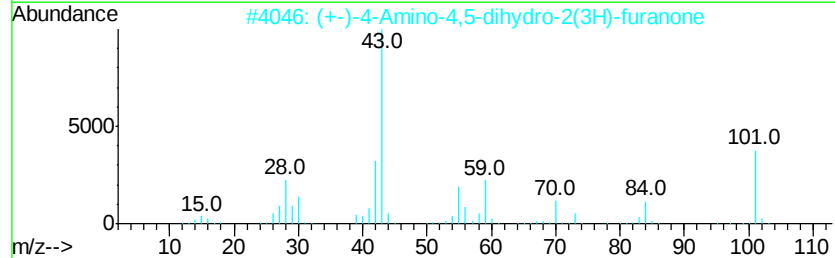
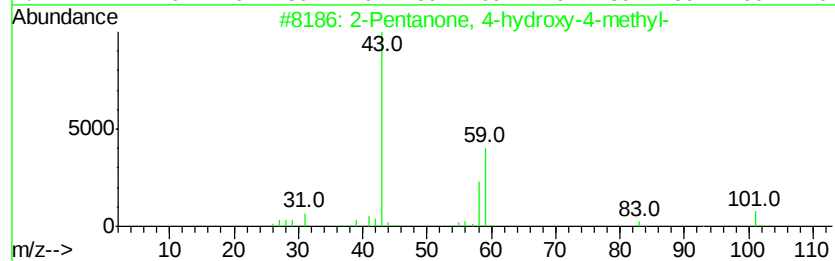
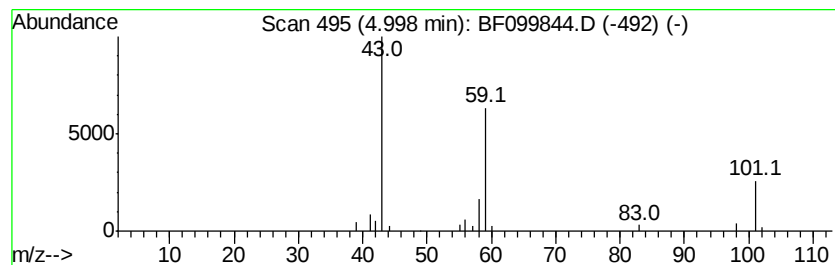
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	3.90 ng	77362	1,4-Dichlorobenzene-d4	6.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	47
3			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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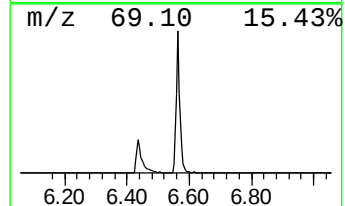
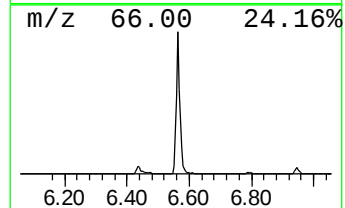
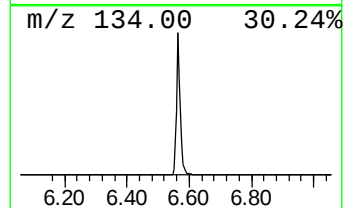
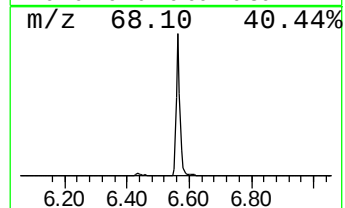
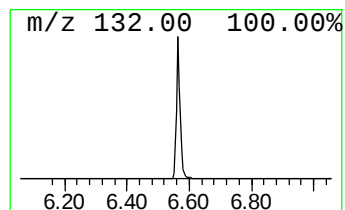
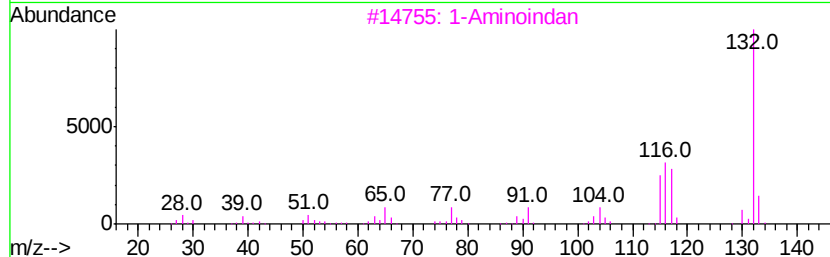
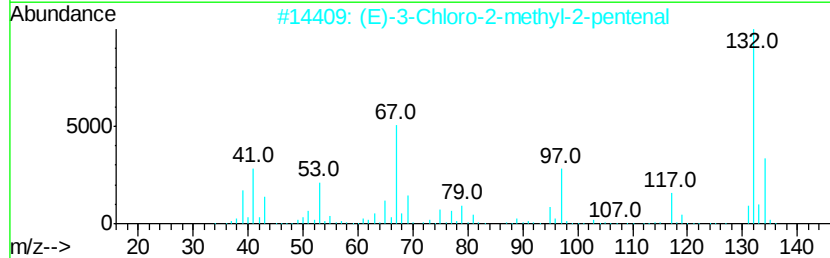
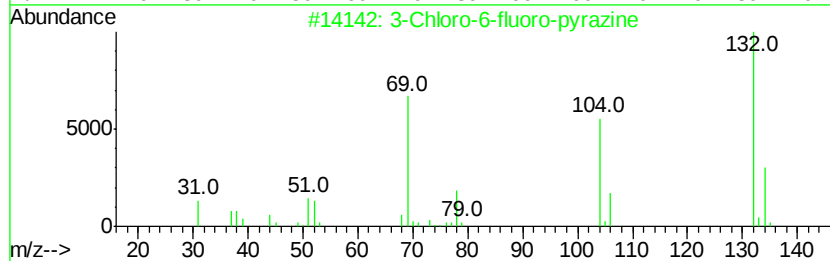
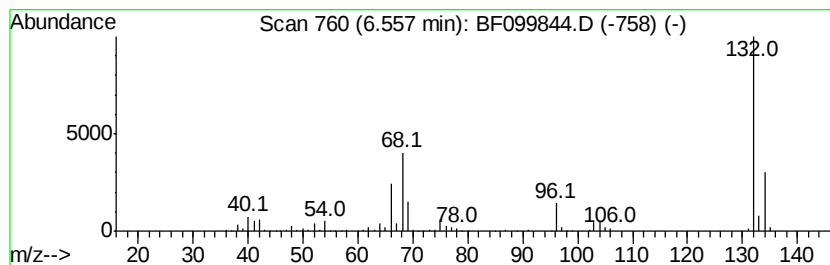
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.56 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	53.09 ng	1052900	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		1-Aminoindan	133	C9H11N	034698-41-4	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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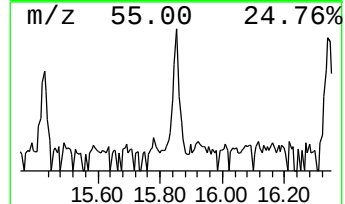
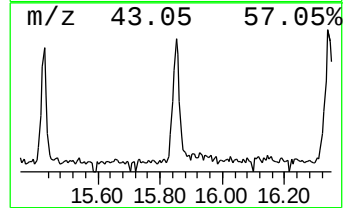
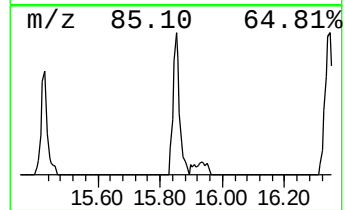
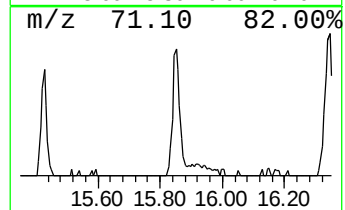
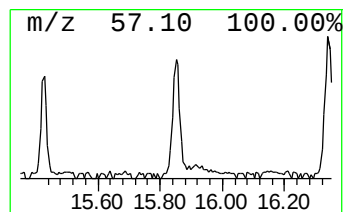
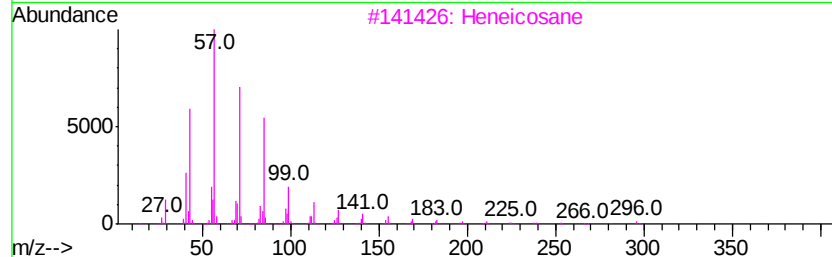
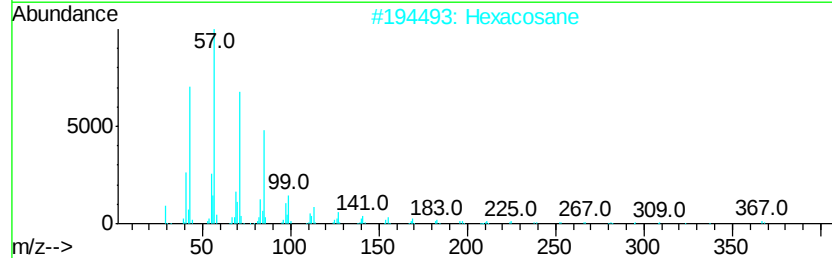
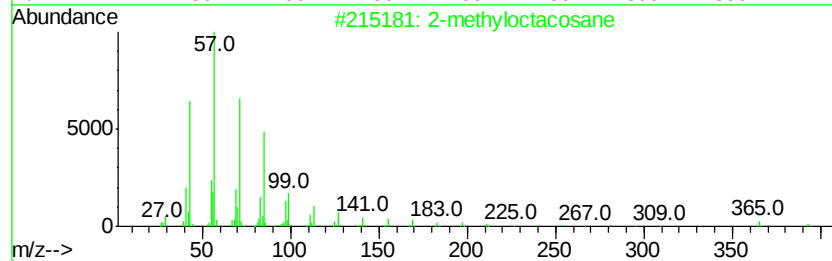
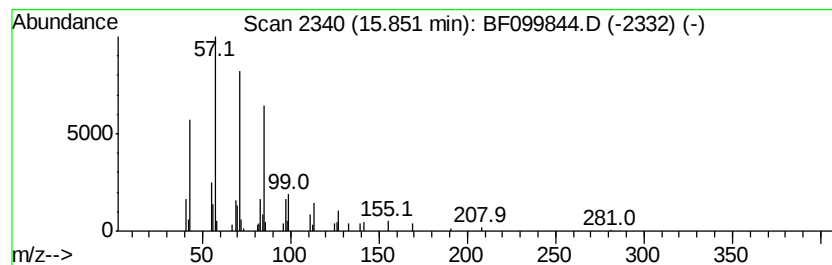
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Peak Number 4 2-methyloctacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.85	3.17 ng	80705	Perylene-d12	15.45

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



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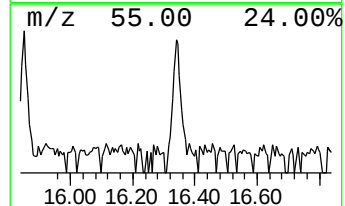
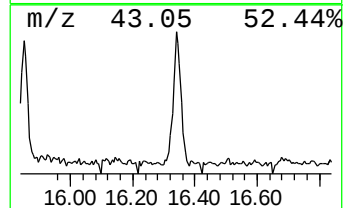
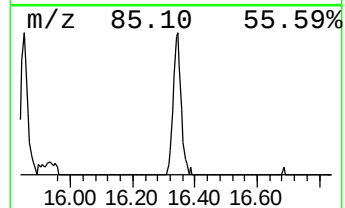
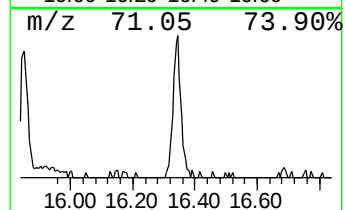
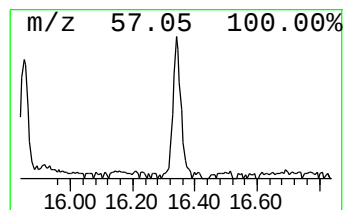
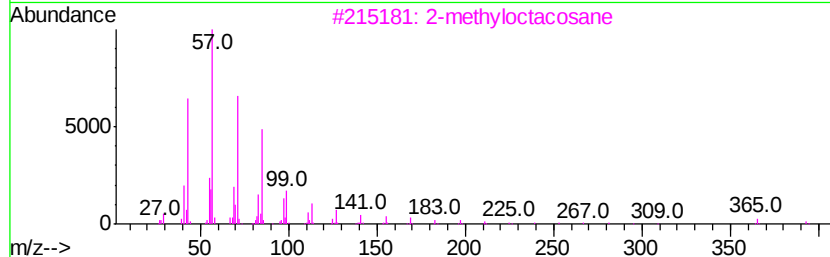
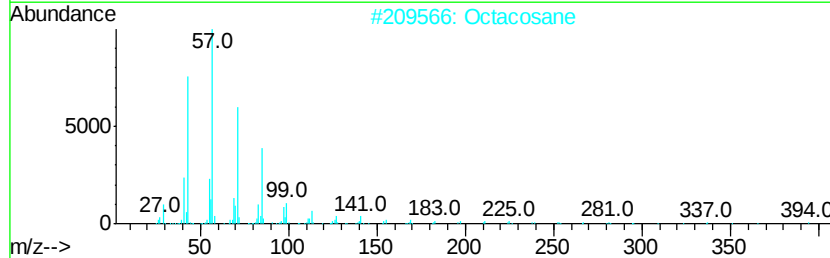
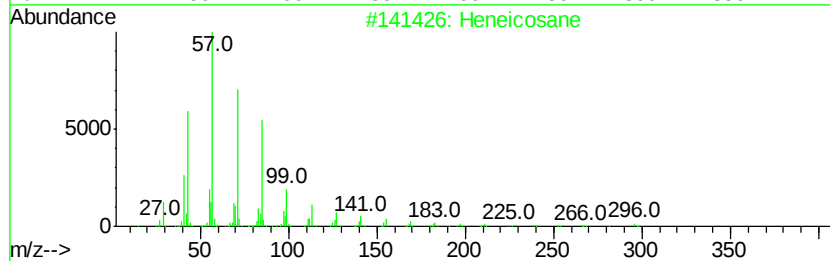
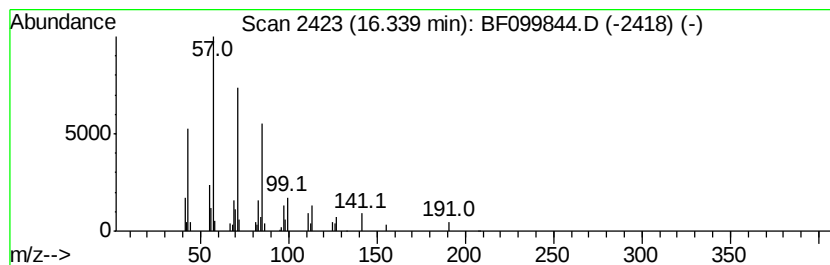
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.34	3.73 ng	95011	Perylene-d12	15.45

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Octacosane		394	C28H58	000630-02-4	91
3	2-methyloctacosane		408	C29H60	1000376-72-8	90
4	Hexacosane		366	C26H54	000630-01-3	87
5	Heptadecane		240	C17H36	000629-78-7	87



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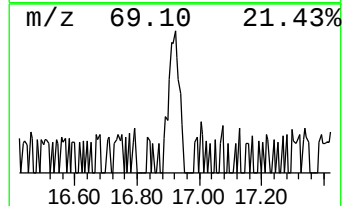
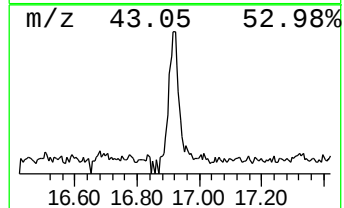
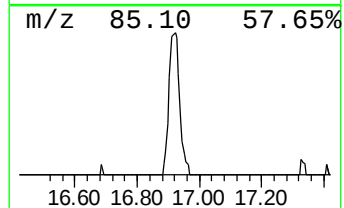
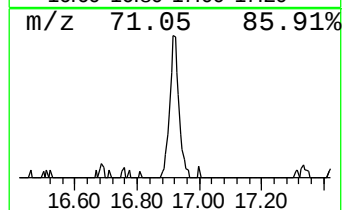
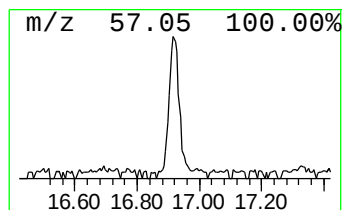
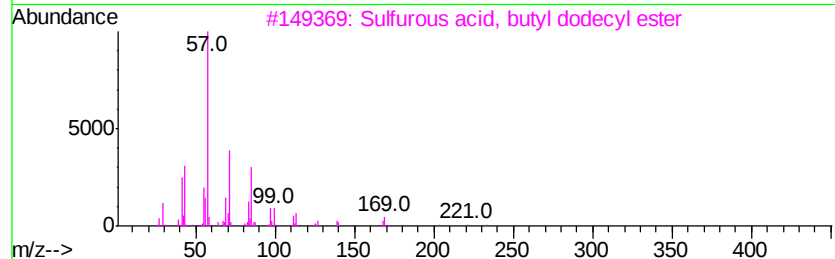
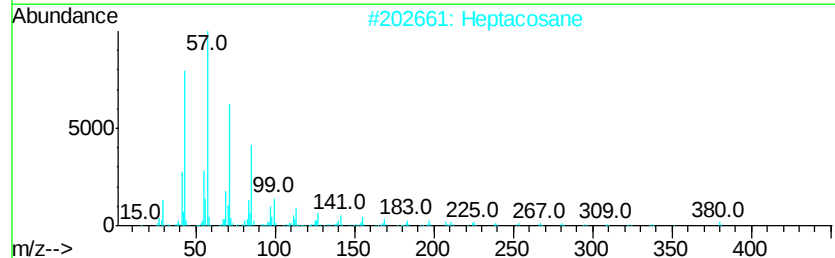
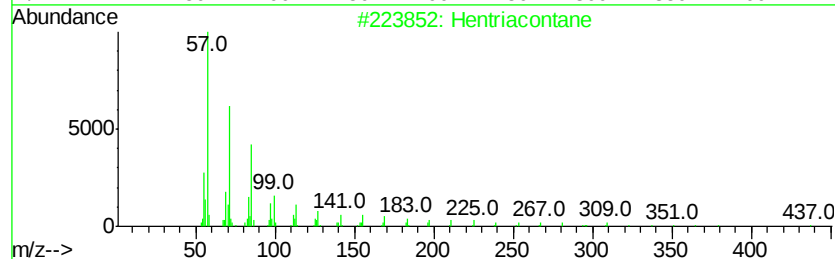
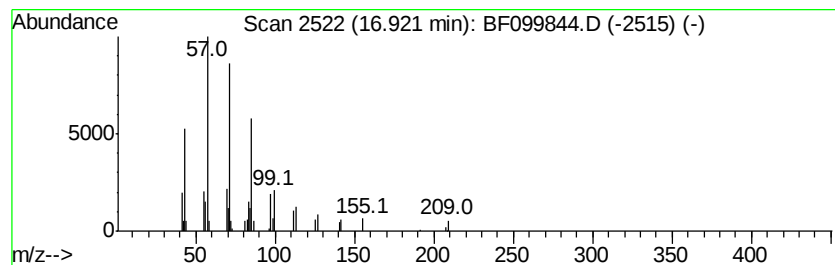
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Hentriacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.92	3.26 ng	82907	Perylene-d12	15.45

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane		437	C31H64	000630-04-6	90
2	Heptacosane		380	C27H56	000593-49-7	90
3	Sulfurous acid, butyl dodecyl ester		306	C16H34O3S	1000309-17-9	90
4	2-methyltetracosane		352	C25H52	1000376-72-6	90
5	Hexacosane		366	C26H54	000630-01-3	87



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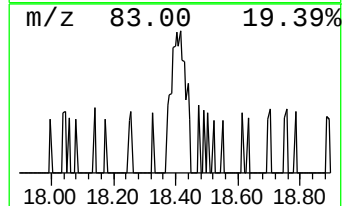
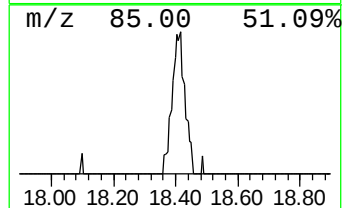
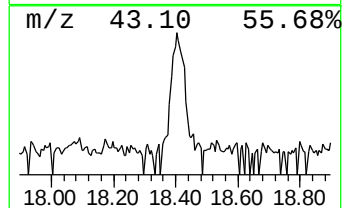
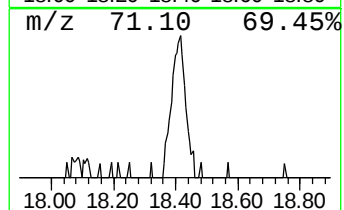
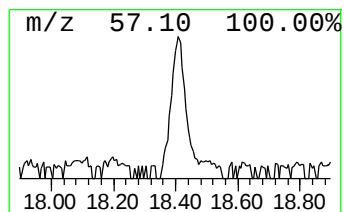
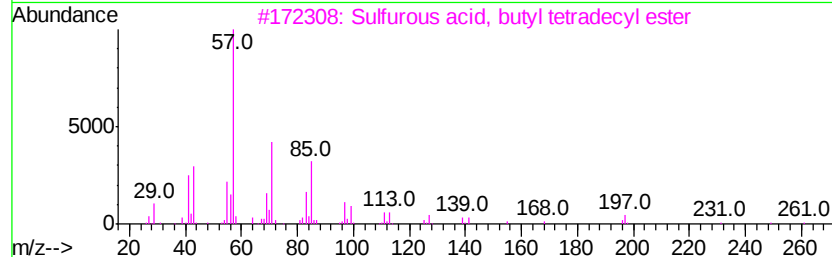
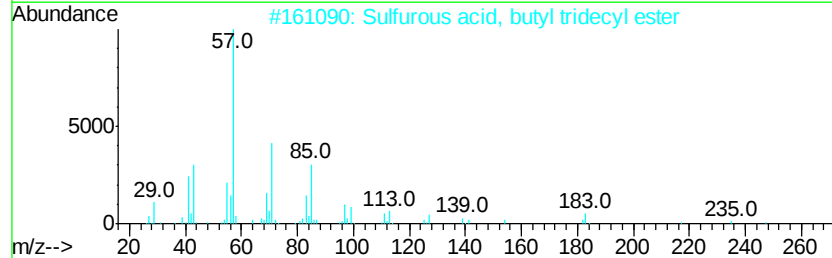
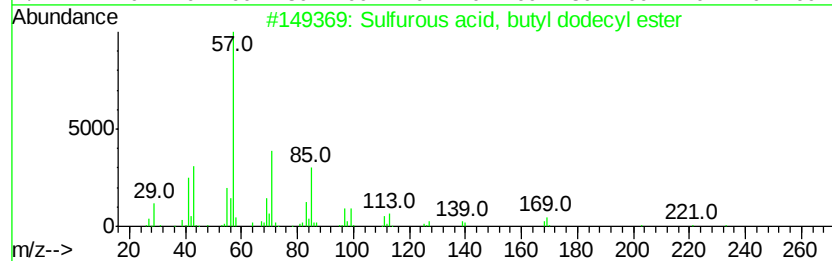
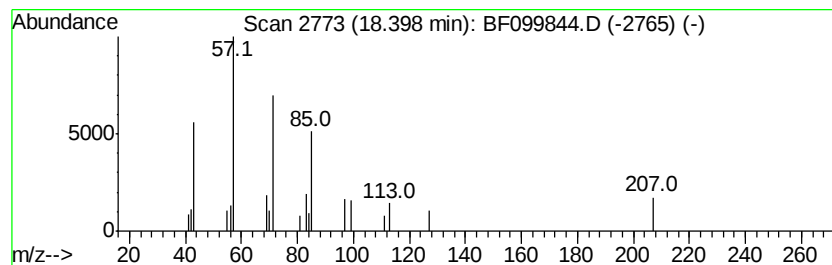
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Sulfurous acid, butyl dodec... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.40	2.35 ng	59785	Perylene-d12	15.45

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	86
2		Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	78
3		Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	78
4		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	72
5		Tetratetracontane	619	C44H90	007098-22-8	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102517\
Data File : BF099844.D
Acq On : 26 Oct 2017 6:35
Operator : SJ/JU
Sample : I6057-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
101917-TIDO-F-U-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.00	3.9	ng	77362	1	6.79	396615	20.0
unknown6.56	6.56	53.1	ng	1052900	1	6.79	396615	20.0
2-methyloctacosane	15.85	3.2	ng	80705	6	15.45	508906	20.0
Heneicosane	16.34	3.7	ng	95011	6	15.45	508906	20.0
Hentriacontane	16.92	3.3	ng	82907	6	15.45	508906	20.0
Sulfurous acid, b...	18.40	2.4	ng	59785	6	15.45	508906	20.0