

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121718\
 Data File : BF111577.D
 Acq On : 18 Dec 2018 9:44
 Operator : JU/SJ
 Sample : PB115763BL
 Misc :
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB115763BL

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-BF121418.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	491	495	507	rVB	114776	158480	5.44%	0.715%
2	5.422	563	567	582	rBV	2811449	2601303	89.30%	11.730%
3	6.434	735	739	757	rBV	2605274	2822518	96.89%	12.728%
4	6.563	757	761	764	rBV	3176698	2759147	94.72%	12.442%
5	6.786	795	799	807	rVB	764767	615834	21.14%	2.777%
6	6.945	821	826	829	rBV	2525436	2140851	73.49%	9.654%
7	7.345	889	894	904	rBV	1649602	1727388	59.30%	7.789%
8	8.069	1012	1017	1023	rBV	829456	734397	25.21%	3.312%
9	9.145	1194	1200	1203	rBV	3483383	2913089	100.00%	13.136%
10	9.822	1311	1315	1324	rBV	790526	720832	24.74%	3.250%
11	10.610	1445	1449	1464	rBV	1307195	1206610	41.42%	5.441%
12	11.304	1563	1567	1578	rBV	600190	553057	18.99%	2.494%
13	12.892	1832	1837	1840	rBV	2208918	1986952	68.21%	8.960%
14	13.939	2012	2015	2030	rVB	499164	517365	17.76%	2.333%
15	15.045	2198	2203	2207	rBV2	37477	43927	1.51%	0.198%
16	15.380	2255	2260	2264	rBV	288892	379102	13.01%	1.709%
17	15.409	2264	2265	2270	rVB	57365	53304	1.83%	0.240%
18	15.833	2332	2337	2343	rVB2	46937	64385	2.21%	0.290%
19	16.321	2414	2420	2429	rVB2	43052	74944	2.57%	0.338%
20	16.886	2509	2516	2524	rBV3	28133	59285	2.04%	0.267%
21	17.568	2626	2632	2637	rVB6	19142	43561	1.50%	0.196%

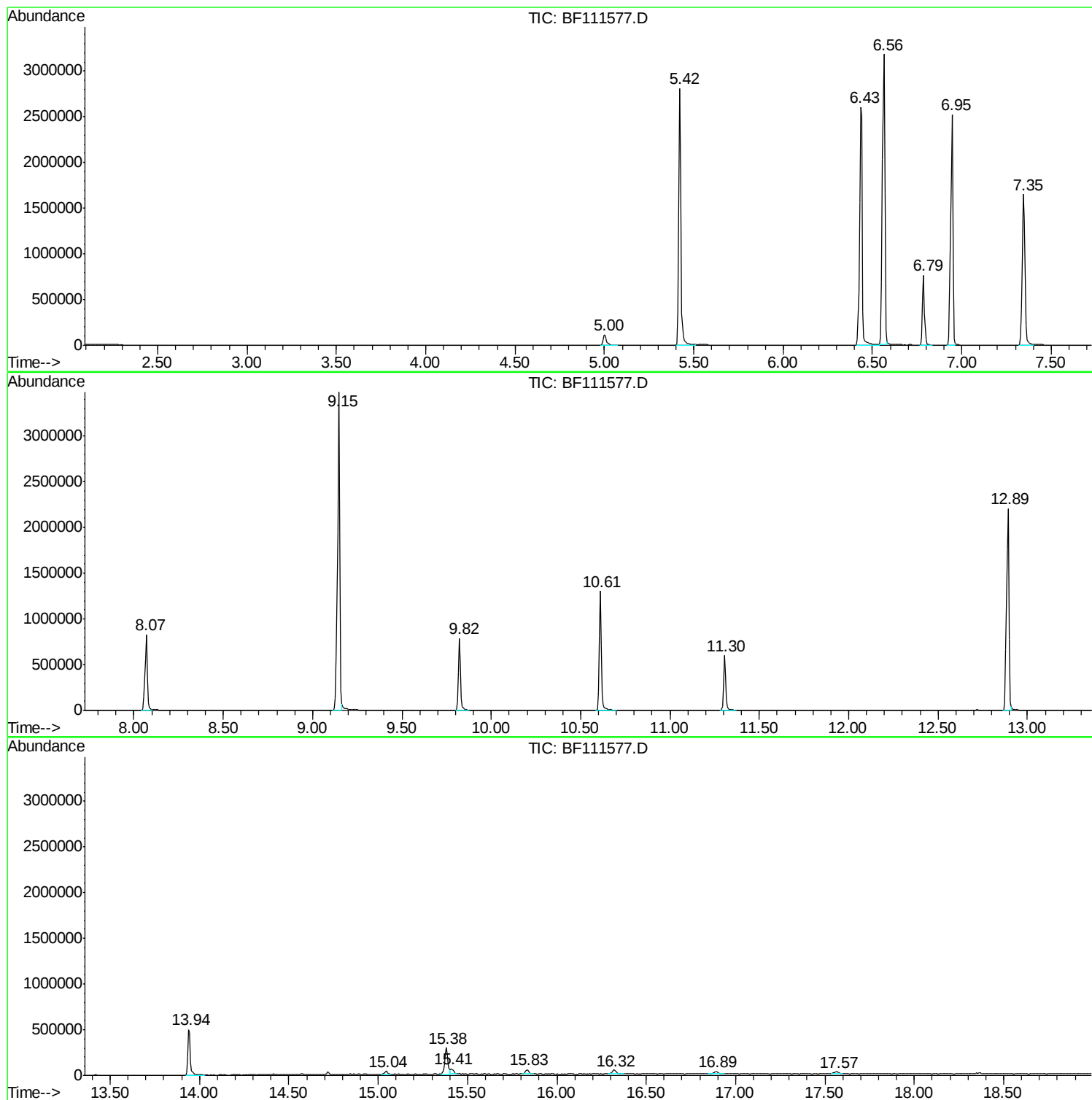
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF121418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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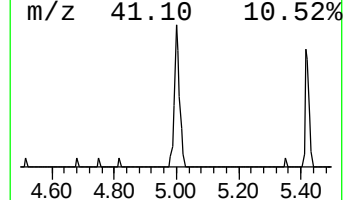
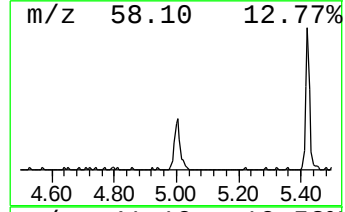
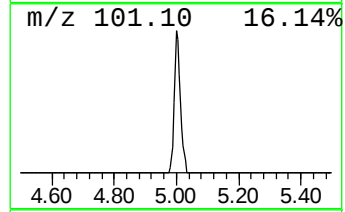
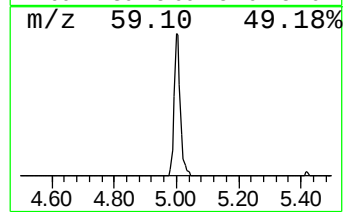
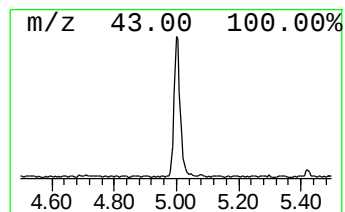
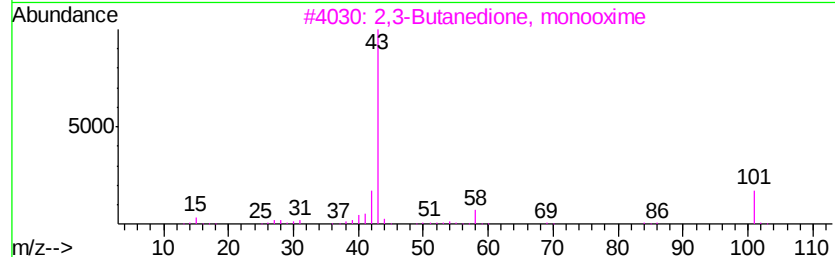
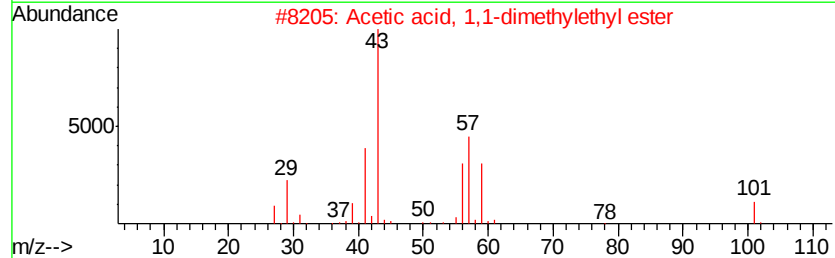
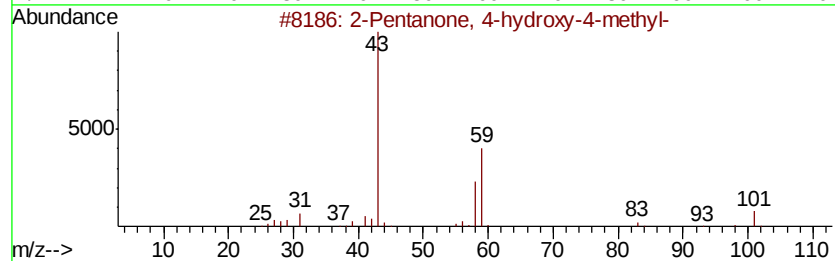
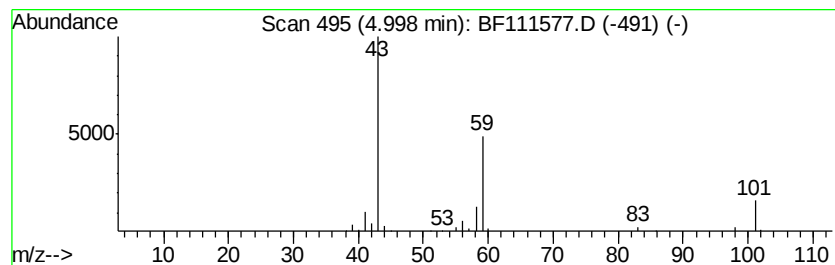
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	5.15 ng	158480	1,4-Dichlorobenzene-d4	6.79

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	28
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5		1-Butene, 4-ethoxy-	100	C6H12O	044611-46-3	9



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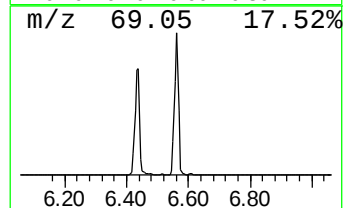
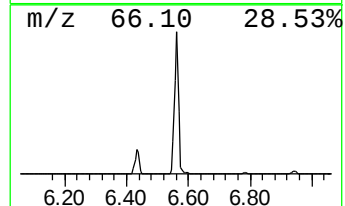
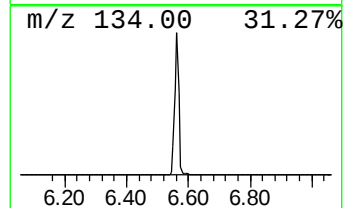
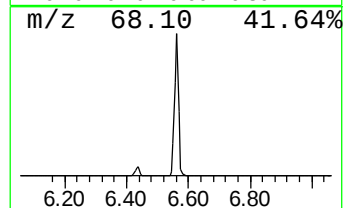
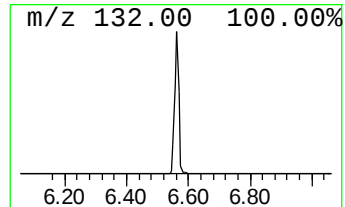
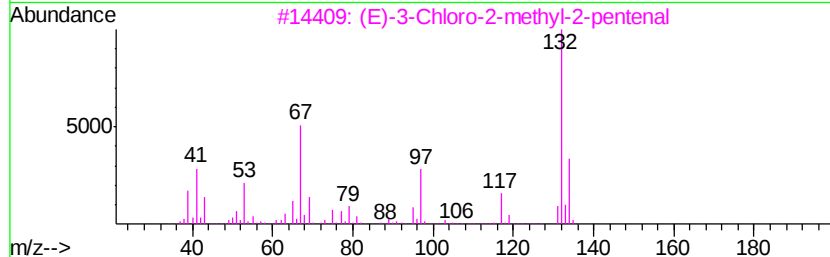
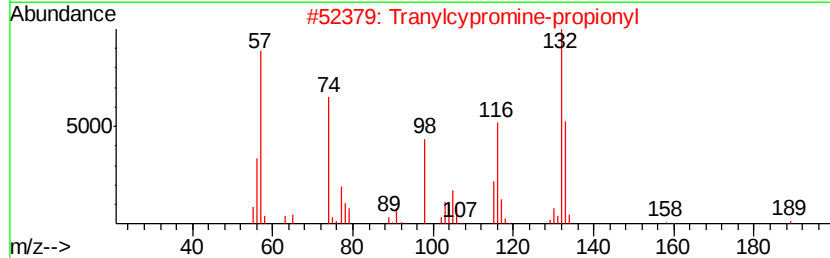
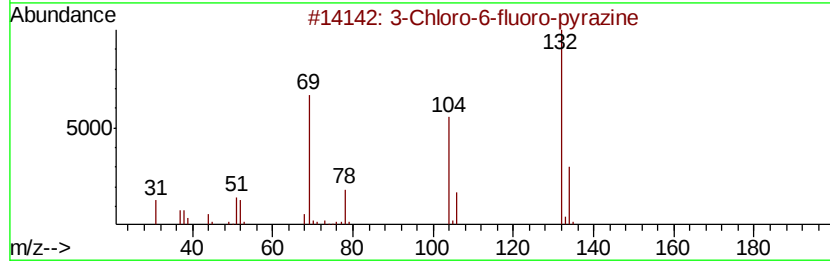
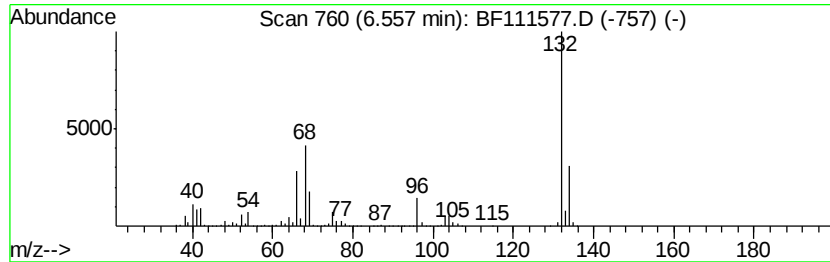
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	89.61 ng	2759150	1,4-Dichlorobenzene-d4	6.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4			2H-Cyclopentadipyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5			1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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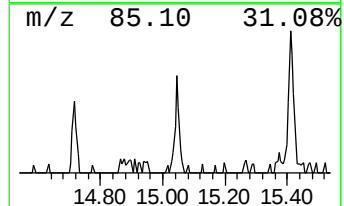
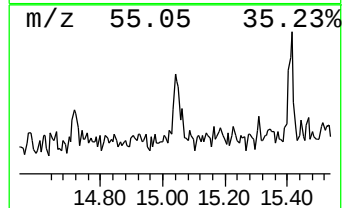
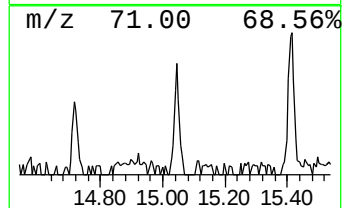
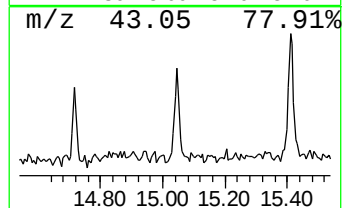
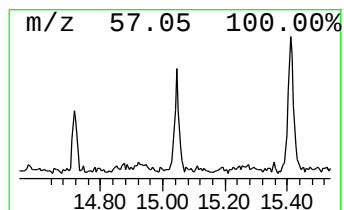
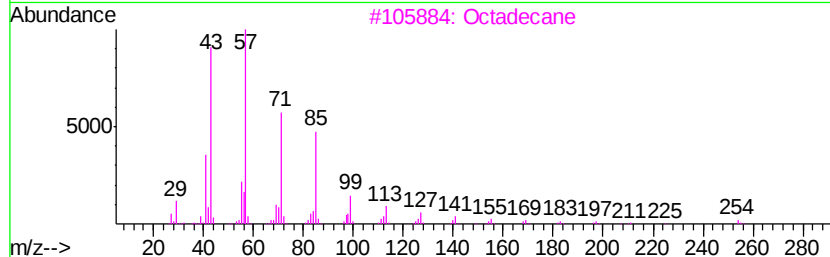
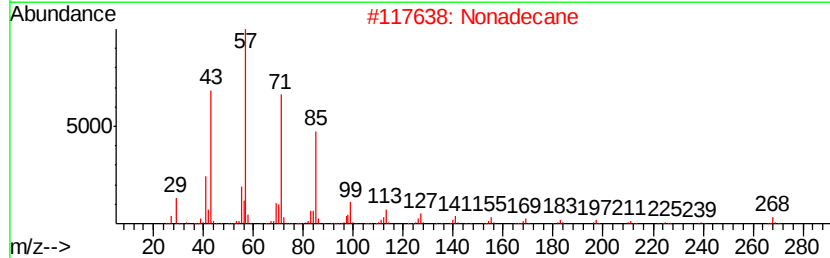
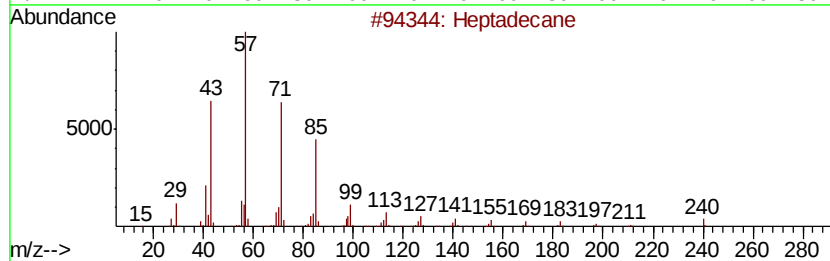
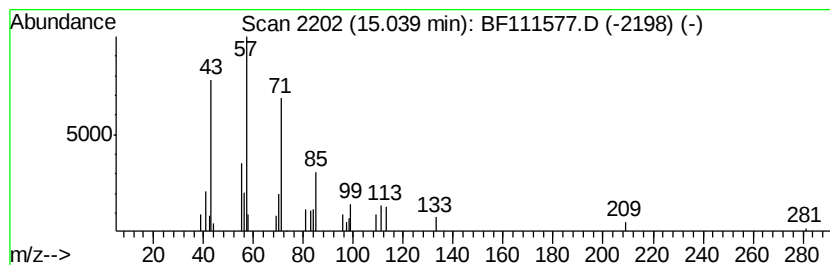
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Peak Number 4 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.04	2.32 ng	43927	Perylene-d12	15.38

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	80
2	Nonadecane		268	C19H40	000629-92-5	80
3	Octadecane		254	C18H38	000593-45-3	80
4	Eicosane		282	C20H42	000112-95-8	80
5	Hexadecane		226	C16H34	000544-76-3	72



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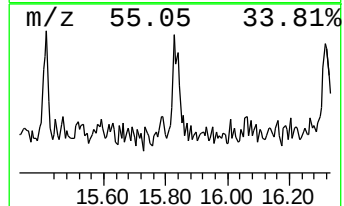
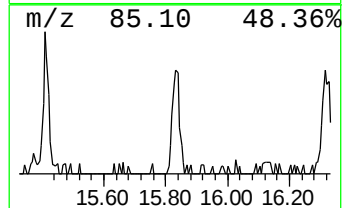
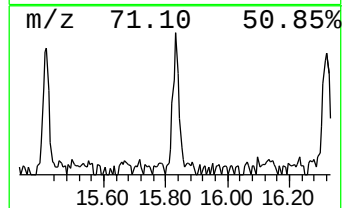
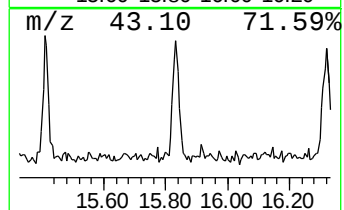
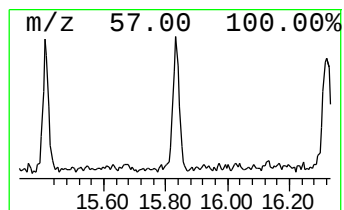
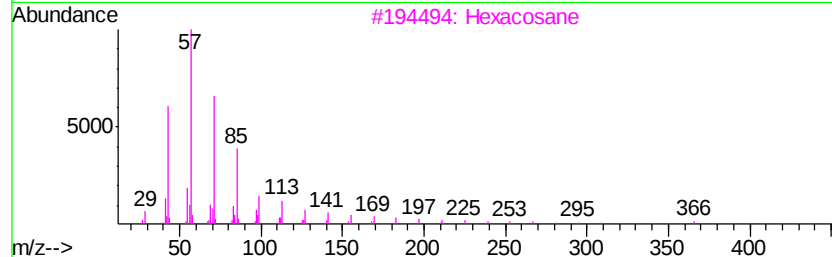
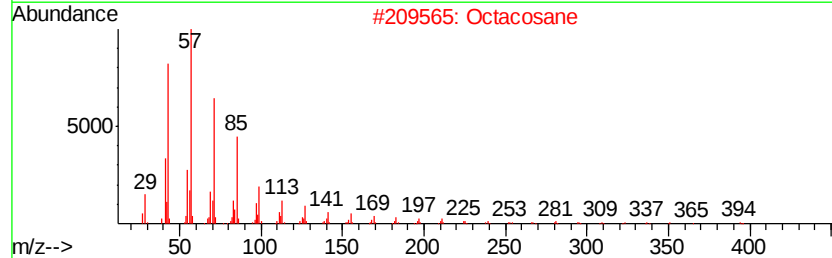
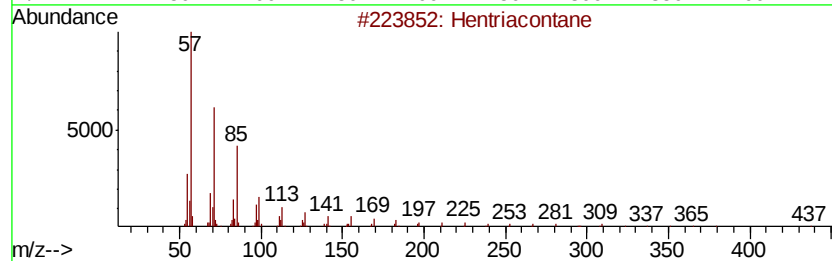
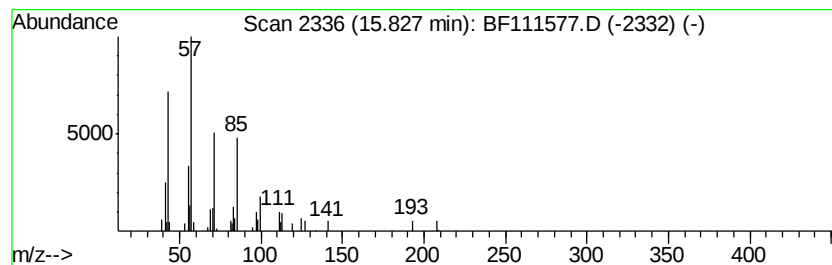
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Peak Number 5 Hentriacontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.83	3.40 ng	64385	Perylene-d12	15.38

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane		437	C31H64	000630-04-6	91
2	Octacosane		394	C28H58	000630-02-4	90
3	Hexacosane		366	C26H54	000630-01-3	90
4	Heptacosane		380	C27H56	000593-49-7	90
5	Heneicosane		296	C21H44	000629-94-7	87



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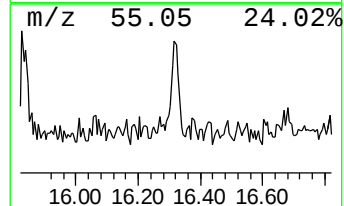
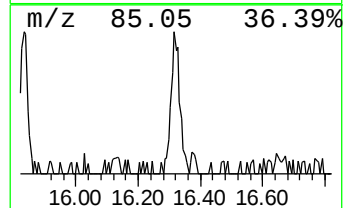
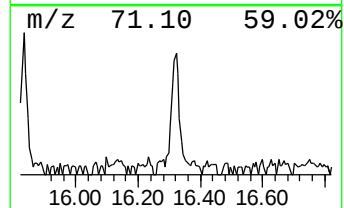
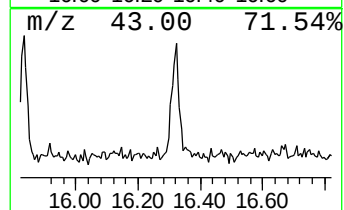
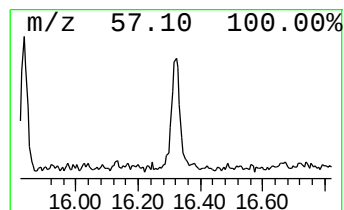
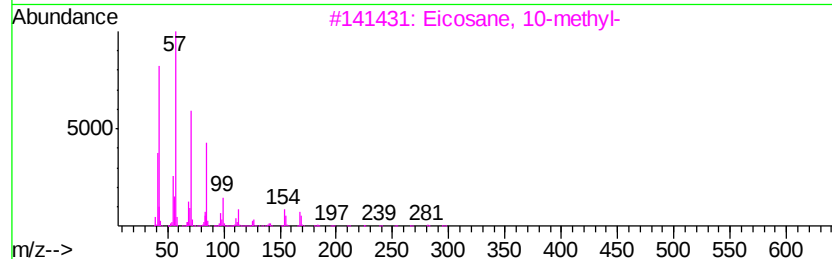
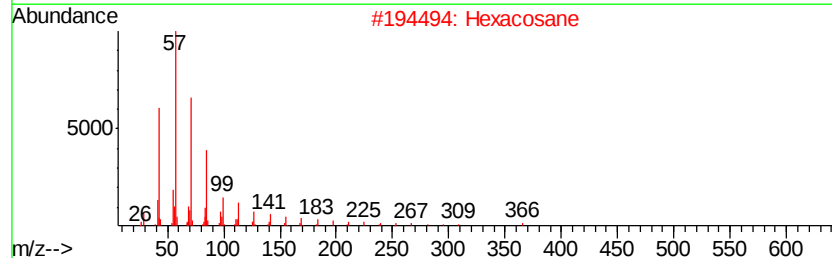
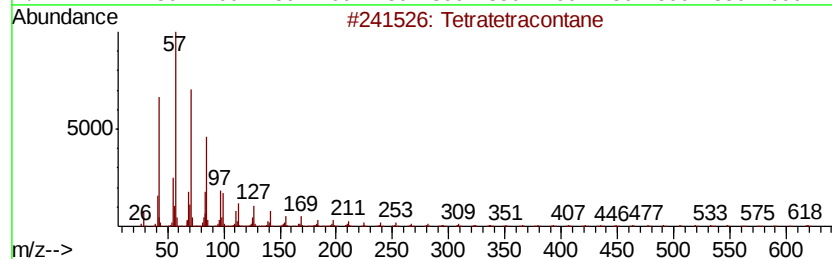
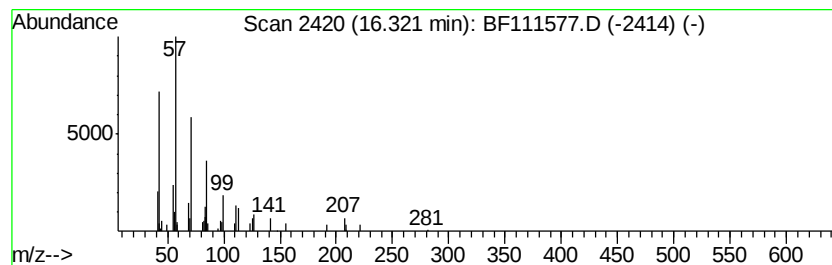
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Tetratetracontane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.32	3.95 ng	74944	Perylene-d12	15.38

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetratetracontane	619	C44H90	007098-22-8	80
2		Hexacosane	366	C26H54	000630-01-3	72
3		Eicosane, 10-methyl-	296	C21H44	054833-23-7	72
4		Hexadecane	226	C16H34	000544-76-3	72
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	72



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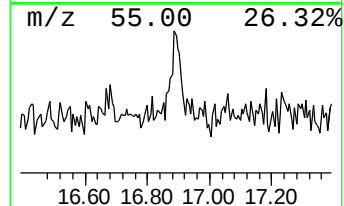
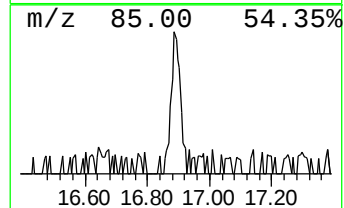
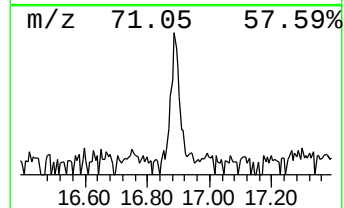
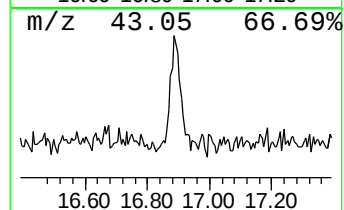
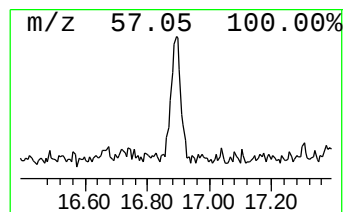
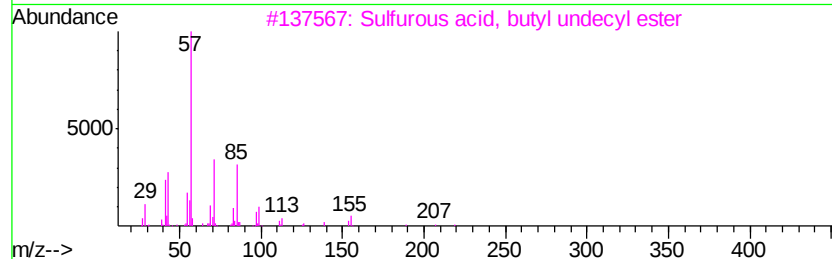
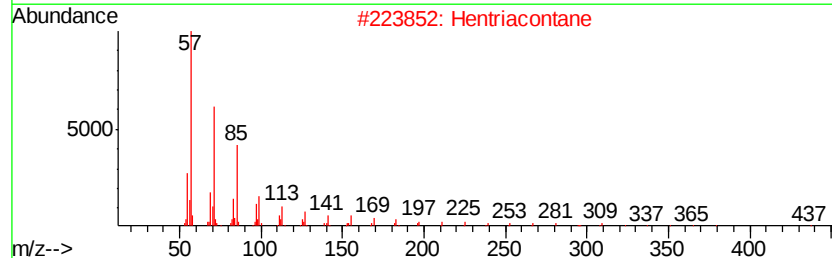
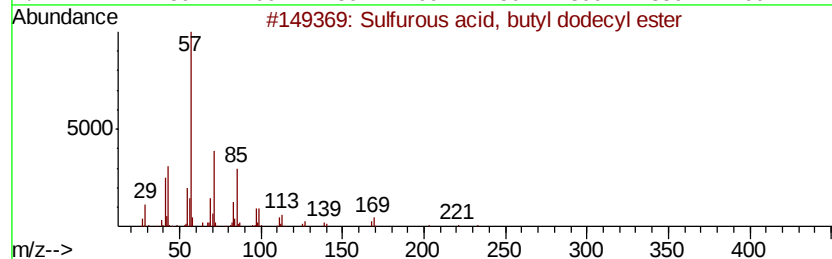
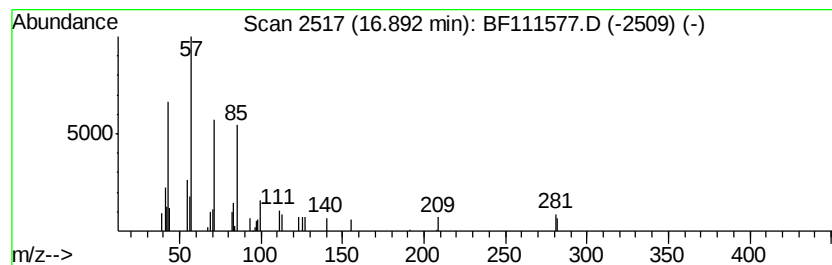
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Sulfurous acid, butyl dodec... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.89	3.13 ng	59285	Perylene-d12	15.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	83
2		Hentriacontane	437	C31H64	000630-04-6	78
3		Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	64
4		Heptacosane	380	C27H56	000593-49-7	64
5		Hexatriacontane	507	C36H74	000630-06-8	59



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121718\
Data File : BF111577.D
Acq On : 18 Dec 2018 9:44
Operator : JU/SJ
Sample : PB115763BL
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB115763BL

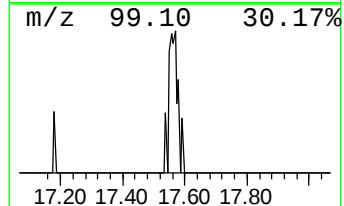
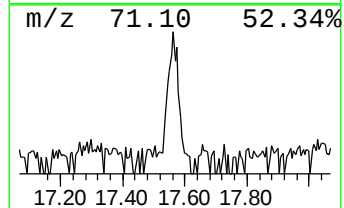
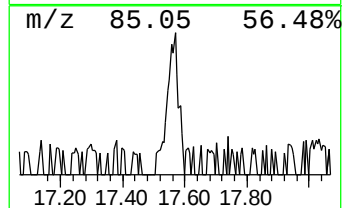
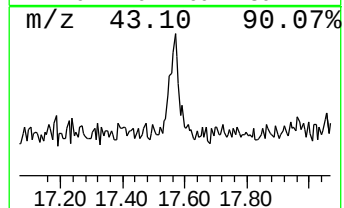
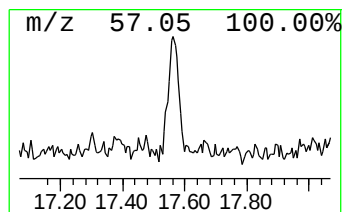
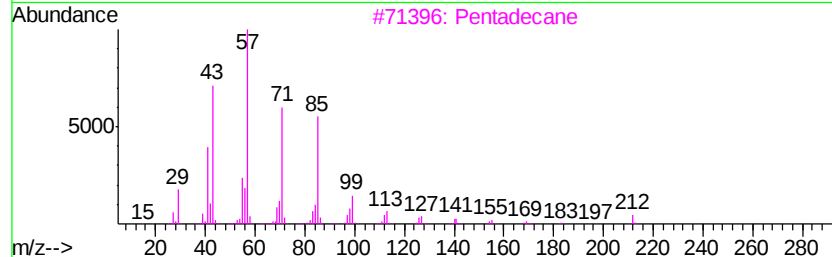
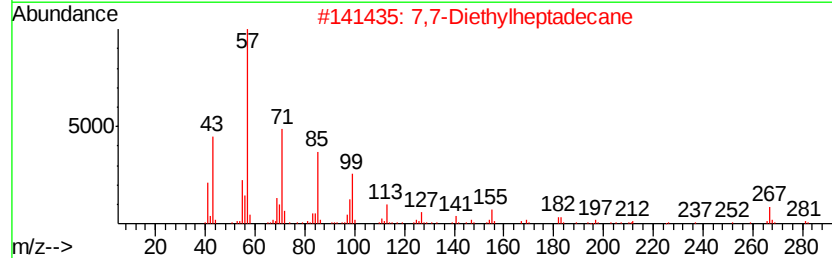
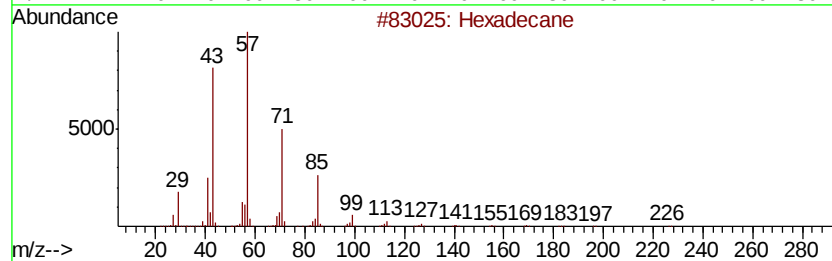
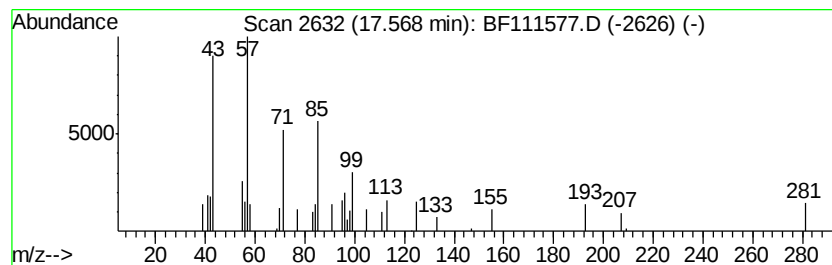
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown17.57 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.57	2.30 ng	43561	Perylene-d12	15.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	43
2		7,7-Diethylheptadecane	296	C21H44	1000360-41-5	43
3		Pentadecane	212	C15H32	000629-62-9	38
4		Nonadecane	268	C19H40	000629-92-5	38
5		Sulfurous acid, hexyl octyl ester	278	C14H30O3S	1000309-13-0	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121718\
Data File : BF111577.D
Acq On : 18 Dec 2018 9:44
Operator : JU/SJ
Sample : PB115763BL
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB115763BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.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	5.2	ng	158480	1	6.79	615834	20.0
unknown6.56	6.56	89.6	ng	2759150	1	6.79	615834	20.0
Heptadecane	15.04	2.3	ng	43927	6	15.38	379102	20.0
Hentriacontane	15.83	3.4	ng	64385	6	15.38	379102	20.0
Tetratetracontane	16.32	4.0	ng	74944	6	15.38	379102	20.0
Sulfurous acid, b...	16.89	3.1	ng	59285	6	15.38	379102	20.0
unknown17.57	17.57	2.3	ng	43561	6	15.38	379102	20.0