

Data Path : U:\HPCHEM1\BNA F\DATA\BF082217\
 Data File : BF097962.D
 Acq On : 22 Aug 2017 19:13
 Operator : SJ/JU
 Sample : PB101741BL
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB101741BL

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-BF081517.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	4.963	485	489	501	rBV	233705	345512	8.65%	1.013%
2	5.369	552	558	561	rBV	3019165	3629246	90.90%	10.637%
3	6.387	724	731	734	rBV	3267976	3644000	91.27%	10.680%
4	6.522	748	754	757	rBV	3079173	3534587	88.53%	10.359%
5	6.745	788	792	796	rBV	1054658	871312	21.82%	2.554%
6	6.904	814	819	822	rBV	2874180	2742317	68.69%	8.037%
7	7.310	883	888	891	rBV	2093443	2375482	59.50%	6.962%
8	8.028	1005	1010	1014	rBV	1271848	1169697	29.30%	3.428%
9	9.110	1187	1194	1197	rBV	3504233	3992494	100.00%	11.701%
10	9.781	1303	1308	1312	rBV2	1390042	1287803	32.26%	3.774%
11	10.569	1436	1442	1446	rBV	2091484	2434628	60.98%	7.136%
12	11.263	1555	1560	1564	rBV	1592648	1390710	34.83%	4.076%
13	12.857	1825	1831	1834	rBV	3574363	3978594	99.65%	11.661%
14	13.898	2003	2008	2011	rBV	1307931	1267477	31.75%	3.715%
15	15.316	2243	2249	2253	rBV	705490	855256	21.42%	2.507%
16	15.357	2253	2256	2262	rVB	51652	67937	1.70%	0.199%
17	15.768	2322	2326	2332	rVB2	58875	82387	2.06%	0.241%
18	16.251	2402	2408	2417	rVB	61610	104348	2.61%	0.306%
19	16.804	2496	2502	2511	rBV2	45120	92359	2.31%	0.271%
20	17.462	2608	2614	2623	rVB3	39328	98951	2.48%	0.290%
21	18.251	2737	2748	2756	rBV3	28273	85850	2.15%	0.252%
22	19.174	2899	2905	2918	rVB8	21277	68615	1.72%	0.201%

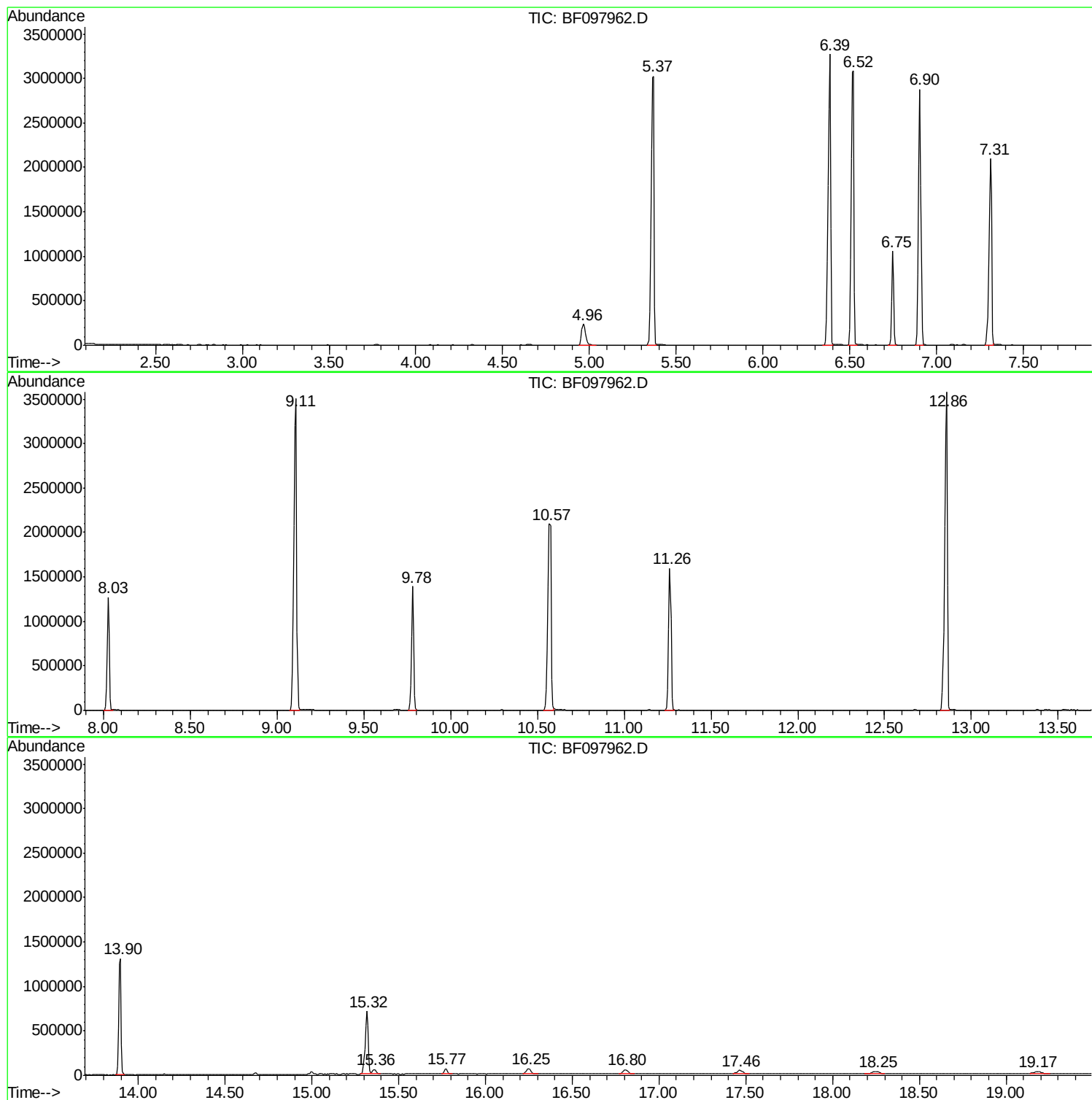
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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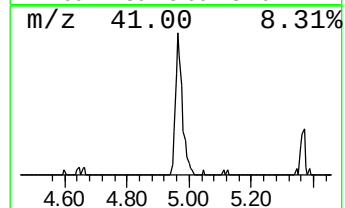
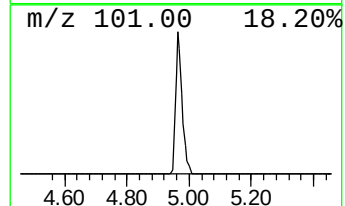
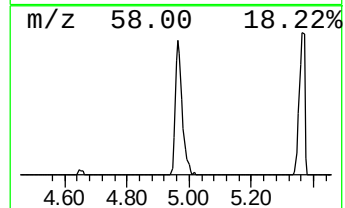
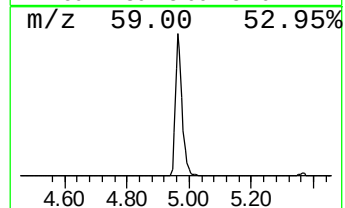
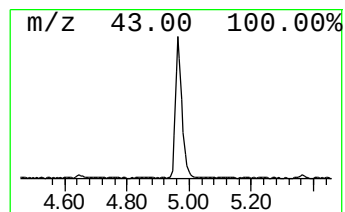
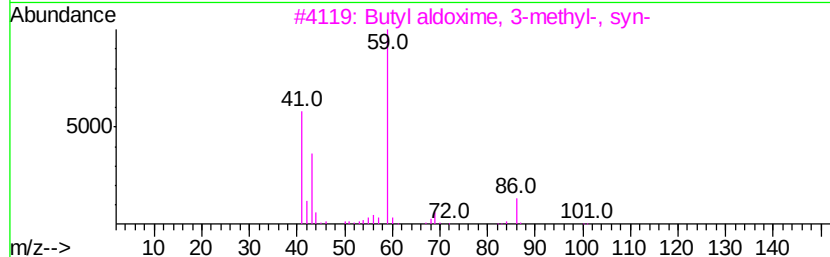
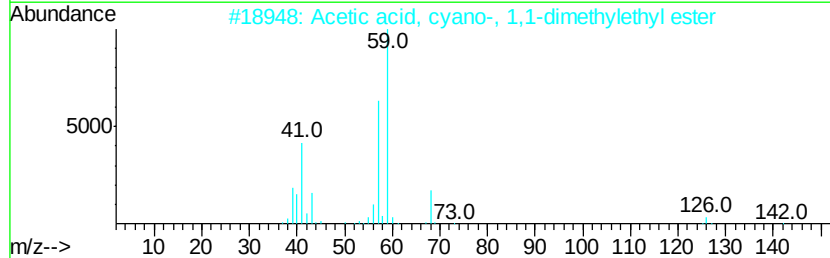
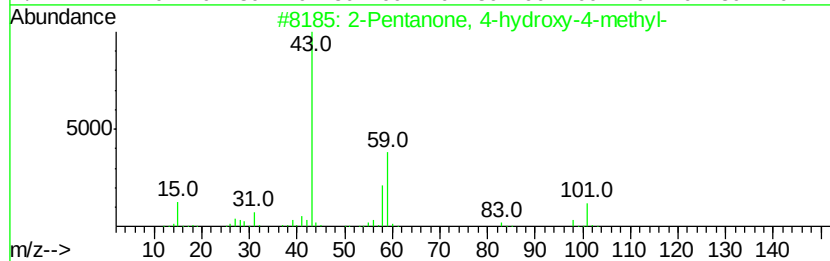
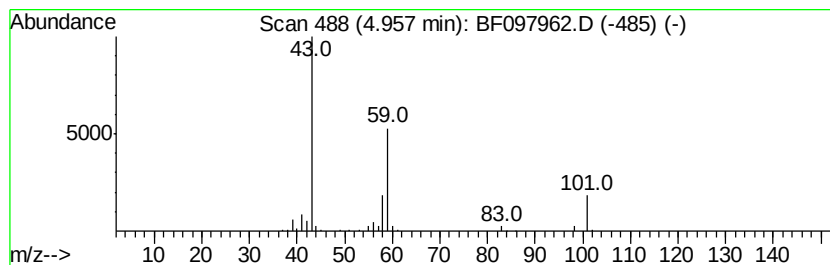
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081517.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	7.93 ng	345512	1,4-Dichlorobenzene-d4	6.75

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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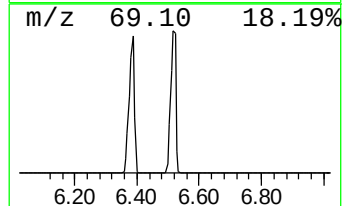
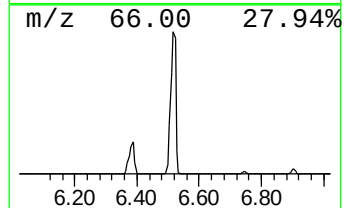
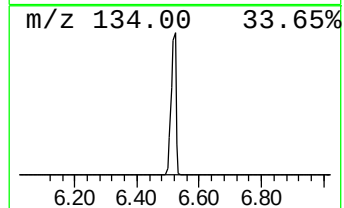
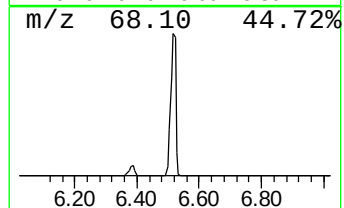
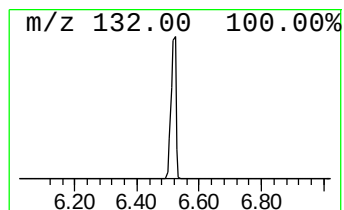
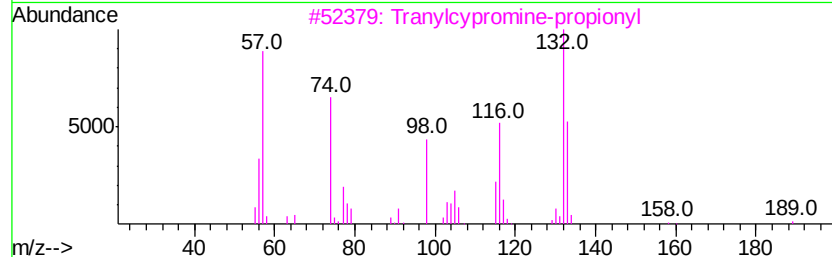
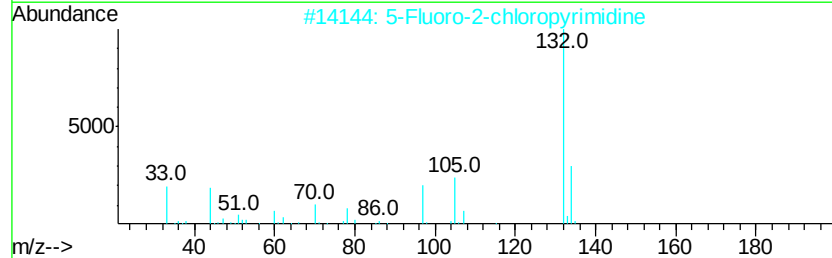
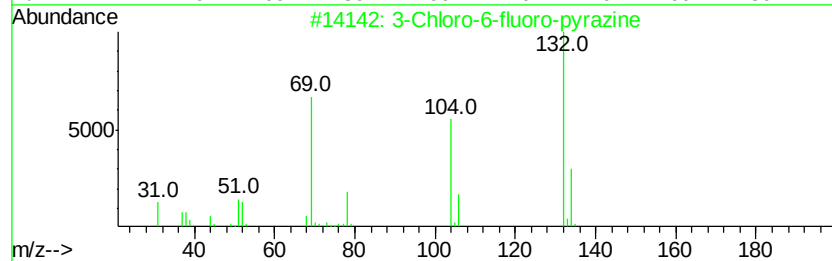
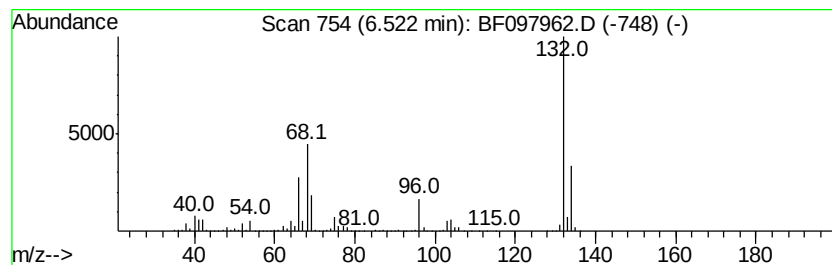
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Peak Number 2 unknown6.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	81.13 ng	3534590	1,4-Dichlorobenzene-d4	6.75

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27		
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12		
3	Tranvlcypromine-propionyl	189	C12H15NO	1000123-86-3	10		
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9		
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9		



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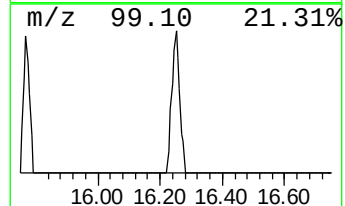
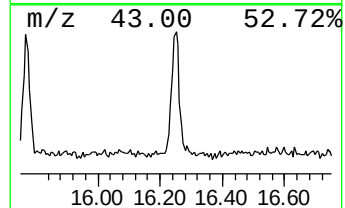
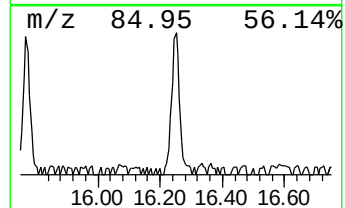
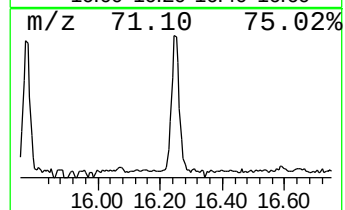
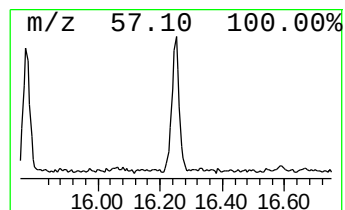
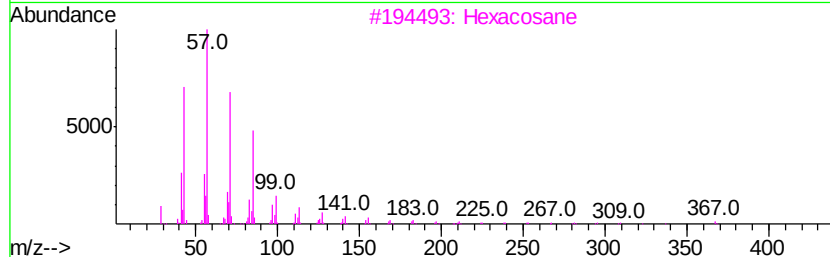
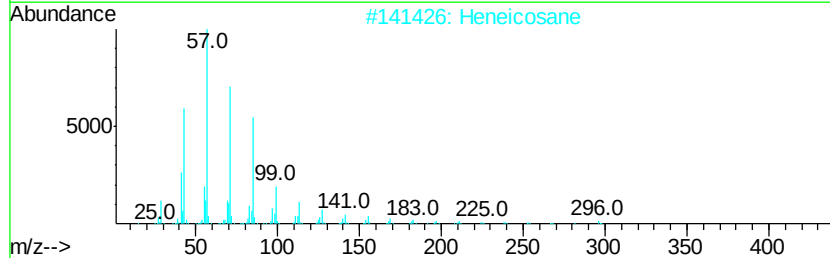
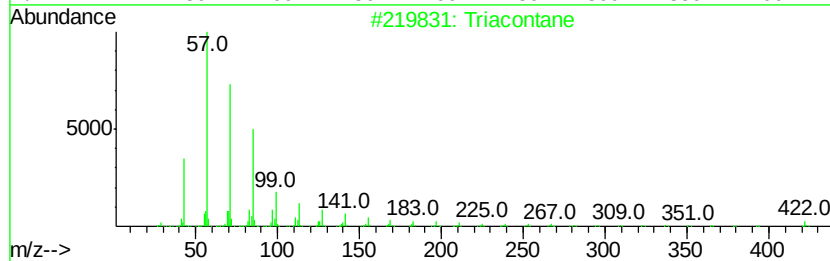
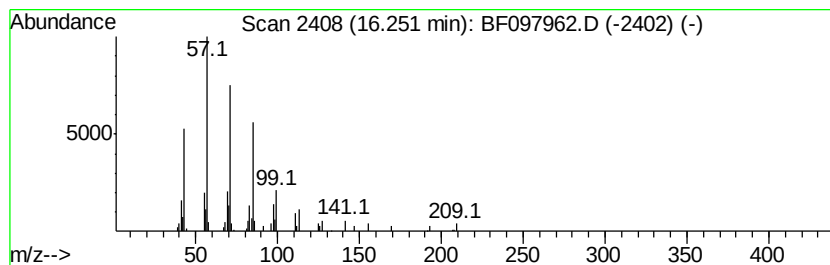
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Peak Number 4 Triacontane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.25	2.44 ng	104348	Perylene-d12	15.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	90
2	Heneicosane	296	C21H44	000629-94-7	87
3	Hexacosane	366	C26H54	000630-01-3	83
4	Heptadecane	240	C17H36	000629-78-7	80
5	Hexadecane	226	C16H34	000544-76-3	80



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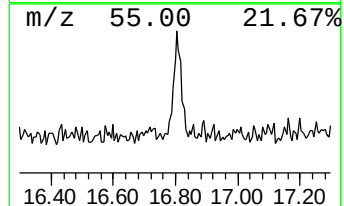
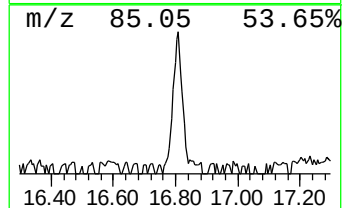
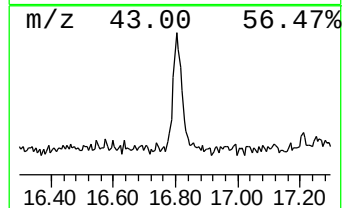
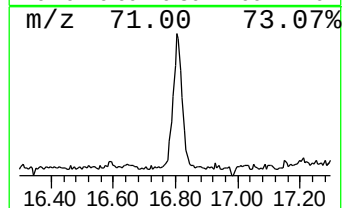
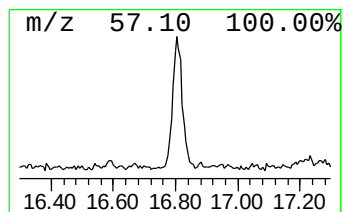
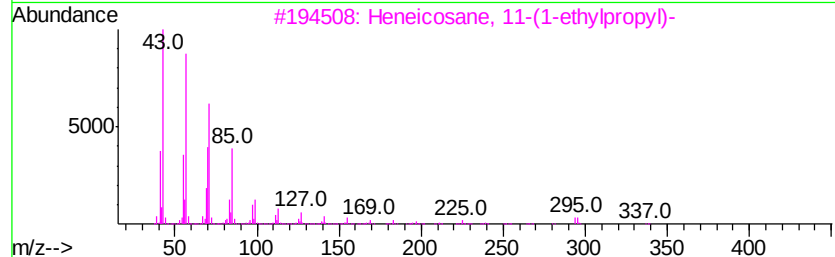
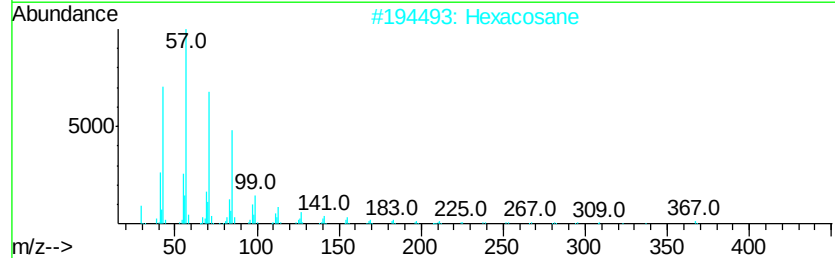
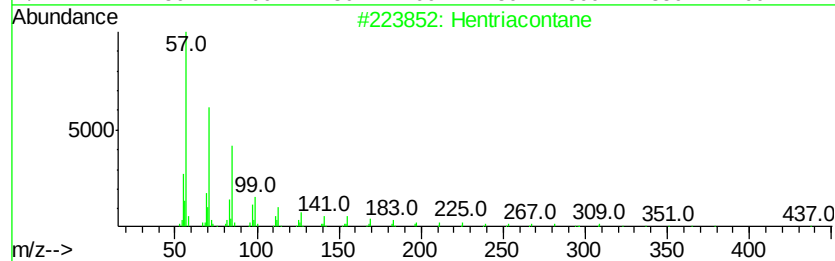
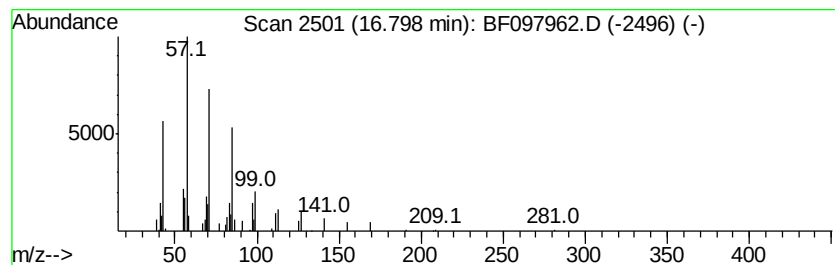
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Peak Number 5 Hentriacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.80	2.16 ng	92359	Perylene-d12	15.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
4	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	90
5	Heptadecane	240	C17H36	000629-78-7	87



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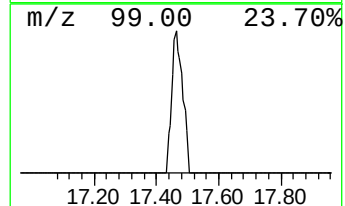
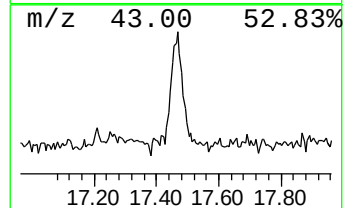
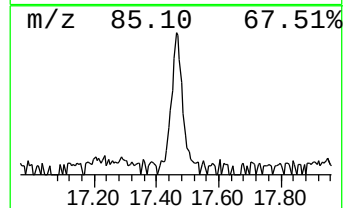
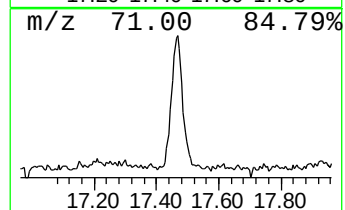
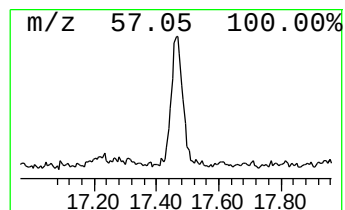
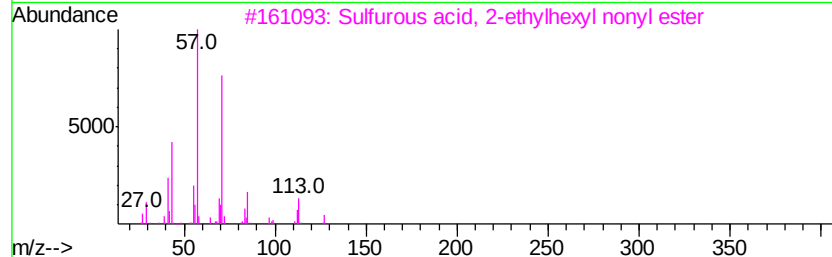
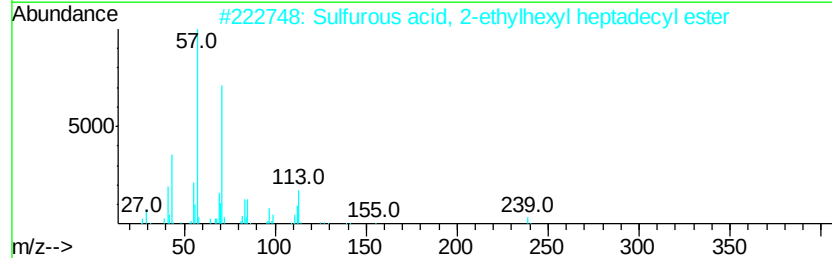
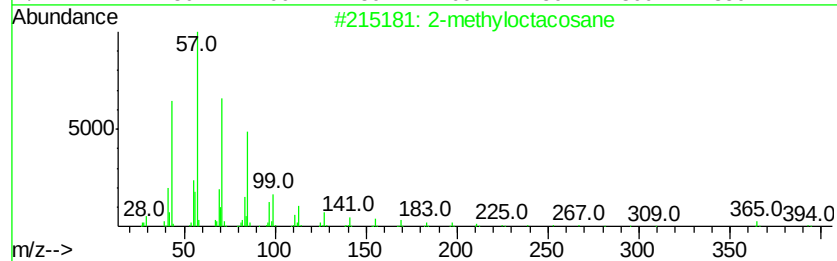
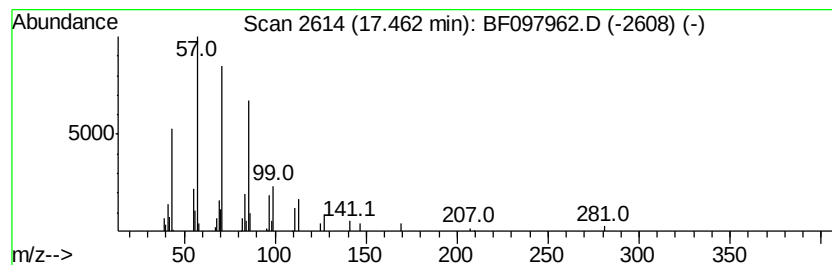
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Peak Number 6 2-methyloctacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.46	2.31 ng	98951	Perylene-d12	15.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	90
2		Sulfurous acid, 2-ethylhexyl hep...	432	C25H52O3S	1000309-20-0	52
3		Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1000309-19-2	49
4		Sulfurous acid, 2-ethylhexyl tet...	390	C22H46O3S	1000309-19-7	47
5		Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	46



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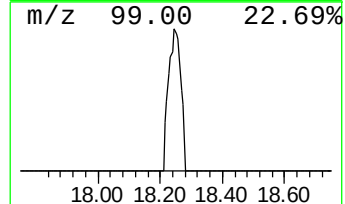
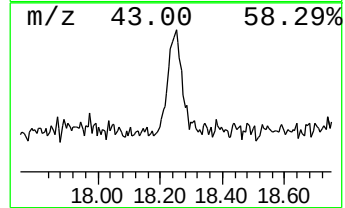
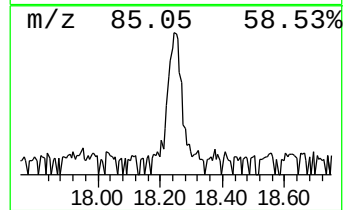
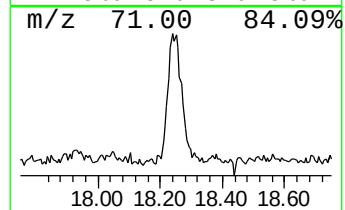
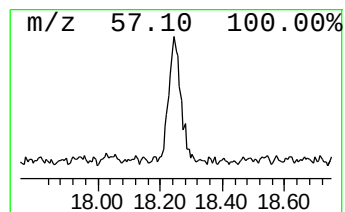
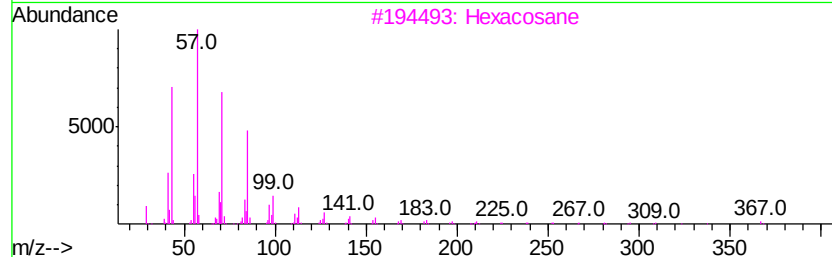
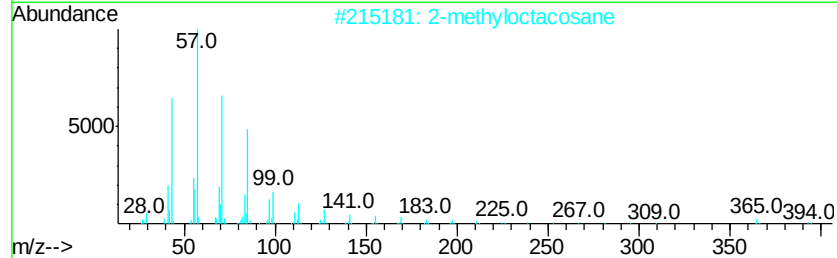
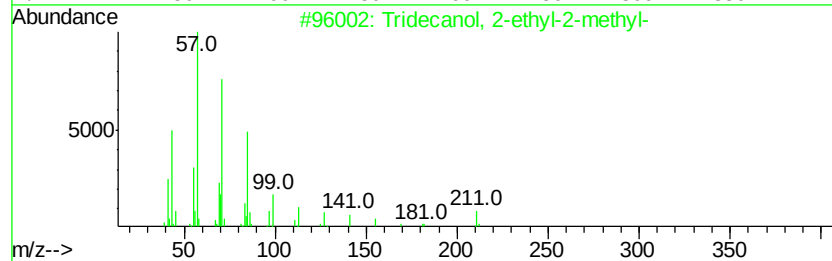
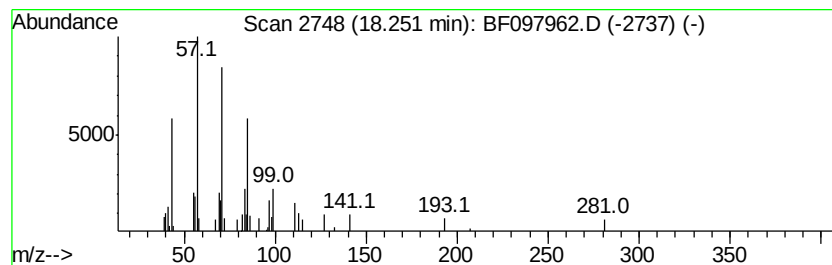
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Tridecanol, 2-ethyl-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.25	2.01 ng	85850	Perylene-d12	15.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	90
2		2-methyloctacosane	408	C29H60	1000376-72-8	86
3		Hexacosane	366	C26H54	000630-01-3	86
4		Tetracosane	338	C24H50	000646-31-1	80
5		Heptadecane	240	C17H36	000629-78-7	80



Data Path : U:\HPCHEM1\BNA_F\DATA\BF082217\
Data File : BF097962.D
Acq On : 22 Aug 2017 19:13
Operator : SJ/JU
Sample : PB101741BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB101741BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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...	4.96	7.9	ng	345512	1	6.75	871312	20.0
unknown6.52	6.52	81.1	ng	3534590	1	6.75	871312	20.0
triacontane	16.25	2.4	ng	104348	6	15.32	855256	20.0
hentriacontane	16.80	2.2	ng	92359	6	15.32	855256	20.0
2-methyloctacosane	17.46	2.3	ng	98951	6	15.32	855256	20.0
tridecanol, 2-eth...	18.25	2.0	ng	85850	6	15.32	855256	20.0