

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062216\
 Data File : BF088260.D
 Acq On : 22 Jun 2016 20:18
 Operator : UM/SJ
 Sample : H3678-02
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TDGA-MH-1617

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-BF060716.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	1.724	11	12	69	rVB	1500688	3450311	100.00%	17.391%
2	4.730	272	275	293	rBV	165387	261006	7.56%	1.316%
3	5.187	313	315	328	rBV	1249306	1399433	40.56%	7.054%
4	6.262	407	409	411	rBV	1163411	1529479	44.33%	7.709%
5	6.364	417	418	421	rBV	1217137	1531018	44.37%	7.717%
6	6.604	437	439	450	rBB	410168	394457	11.43%	1.988%
7	6.753	450	452	455	rBV	1373636	1259928	36.52%	6.351%
8	7.176	487	489	491	rBV	1040726	1039703	30.13%	5.241%
9	7.885	550	551	554	rBV	572120	622933	18.05%	3.140%
10	8.970	643	646	648	rBV	2016065	2089456	60.56%	10.532%
11	9.370	679	681	683	rBV	111045	86577	2.51%	0.436%
12	9.633	702	704	707	rBV	758565	710684	20.60%	3.582%
13	10.422	771	773	776	rBV	1052999	969352	28.09%	4.886%
14	10.548	782	784	789	rVB	32625	38813	1.12%	0.196%
15	11.119	832	834	836	rBV	502390	689652	19.99%	3.476%
16	12.697	969	972	974	rBV	1931820	1864667	54.04%	9.399%
17	13.599	1049	1051	1059	rBV	33070	84438	2.45%	0.426%
18	13.737	1061	1063	1069	rVV	503143	648114	18.78%	3.267%
19	13.919	1076	1079	1081	rBV	34820	35808	1.04%	0.180%
20	14.217	1103	1105	1110	rBV3	25819	53423	1.55%	0.269%
21	14.594	1134	1138	1141	rBV2	26450	56286	1.63%	0.284%
22	14.960	1167	1170	1172	rBV	56362	69779	2.02%	0.352%
23	15.108	1180	1183	1189	rBV	345846	464256	13.46%	2.340%
24	15.371	1203	1206	1210	rVB	77835	125416	3.63%	0.632%
25	15.851	1245	1248	1251	rBV	60485	118692	3.44%	0.598%
26	16.434	1293	1299	1302	rBV2	27376	64831	1.88%	0.327%
27	17.131	1355	1360	1369	rVB	21527	65655	1.90%	0.331%
28	17.988	1430	1435	1441	rVB2	19311	61720	1.79%	0.311%
29	19.040	1521	1527	1534	rBV3	11941	53832	1.56%	0.271%

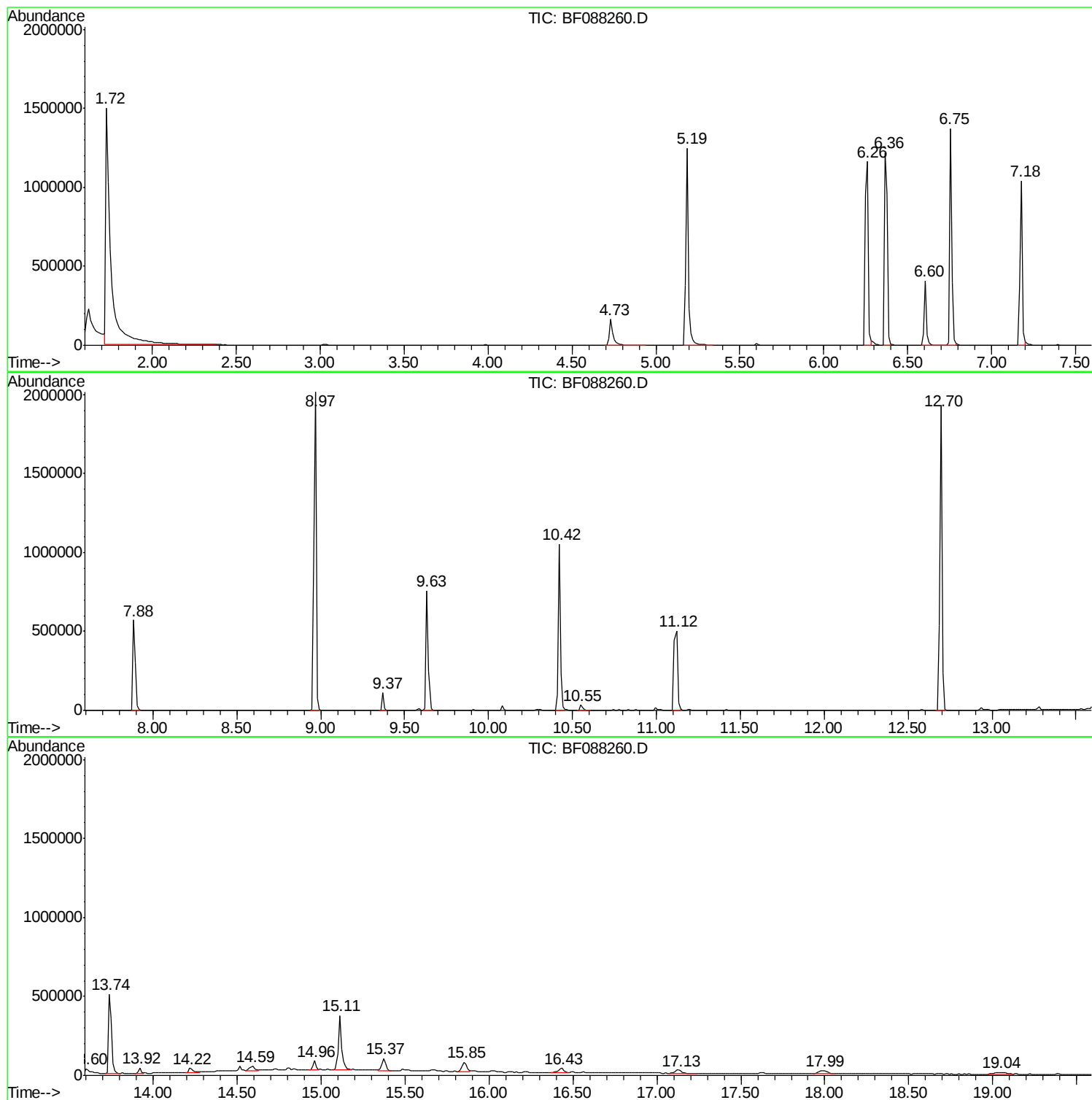
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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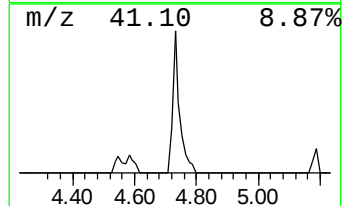
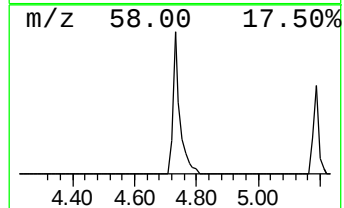
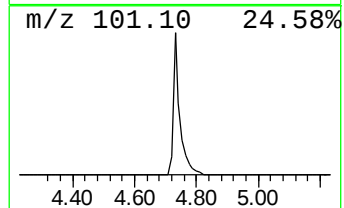
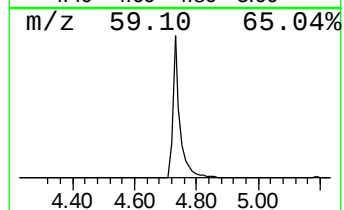
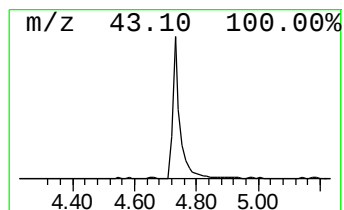
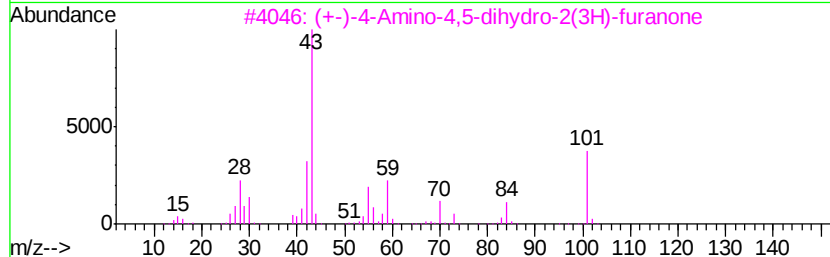
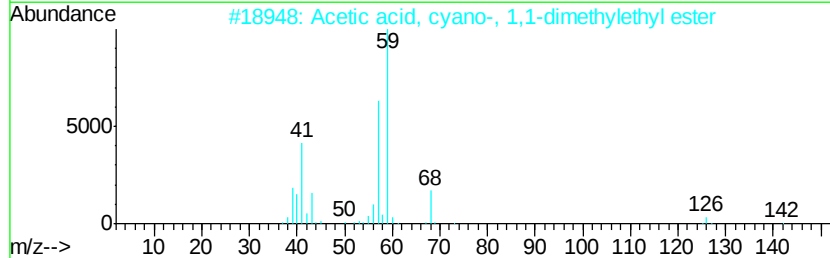
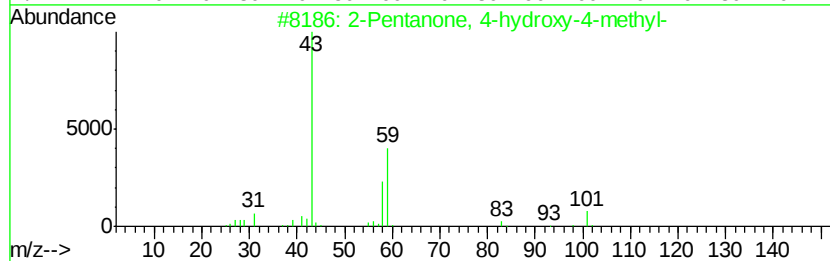
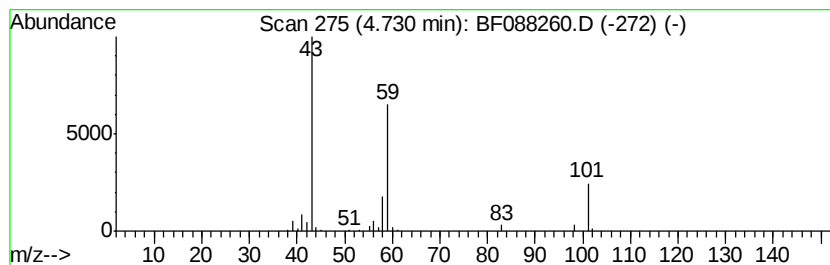
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.73	13.23 ng	261006	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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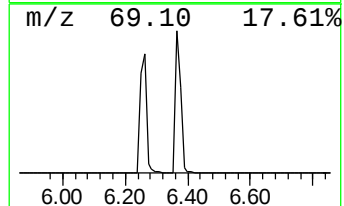
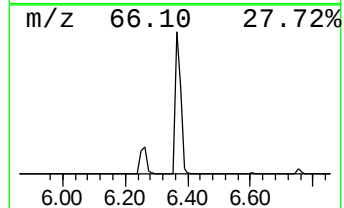
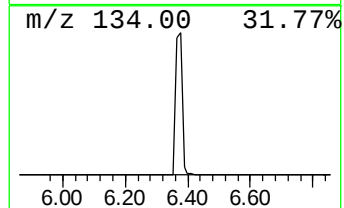
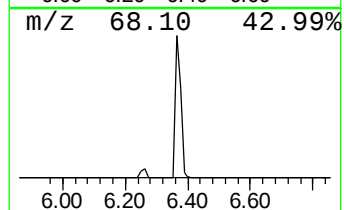
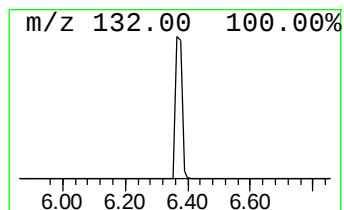
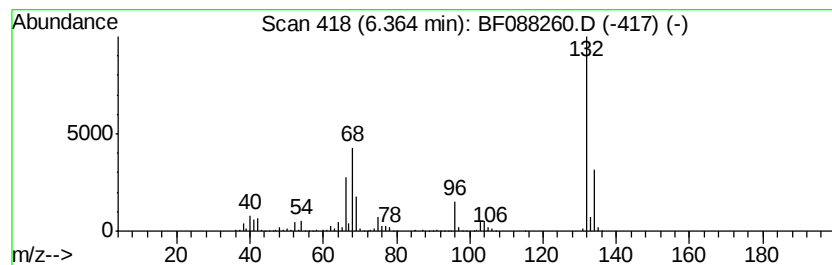
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Peak Number 3 unknown6.36 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.36	77.63 ng	1531020	1,4-Dichlorobenzene-d4	6.60

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4			4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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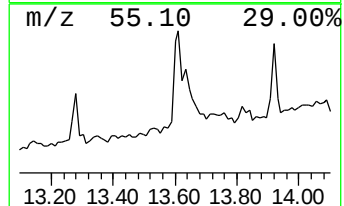
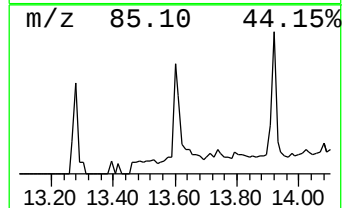
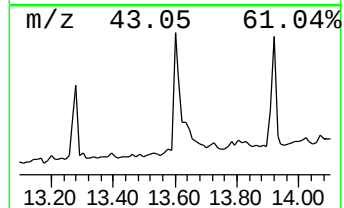
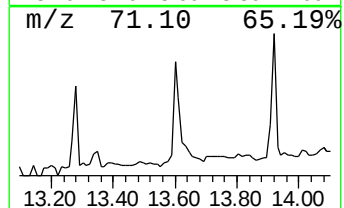
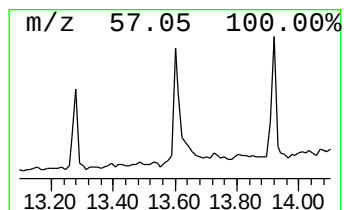
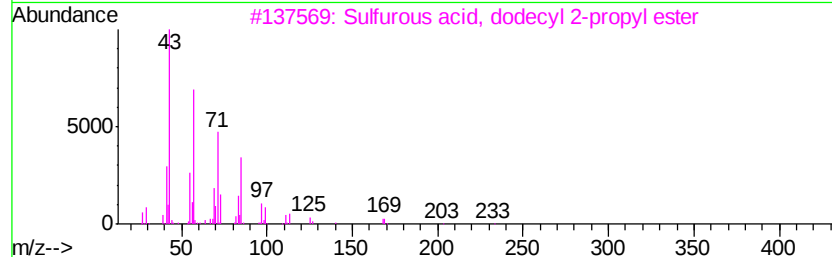
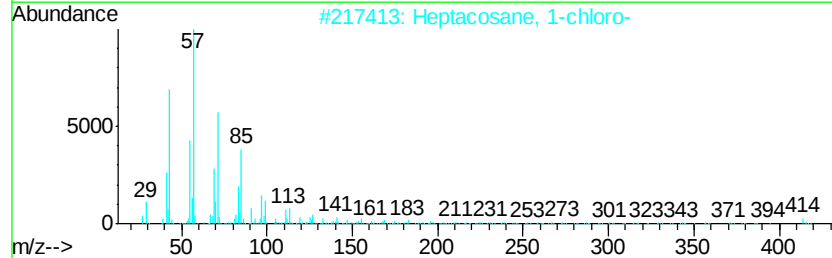
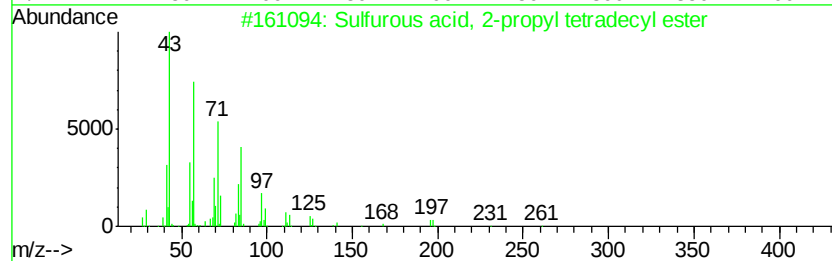
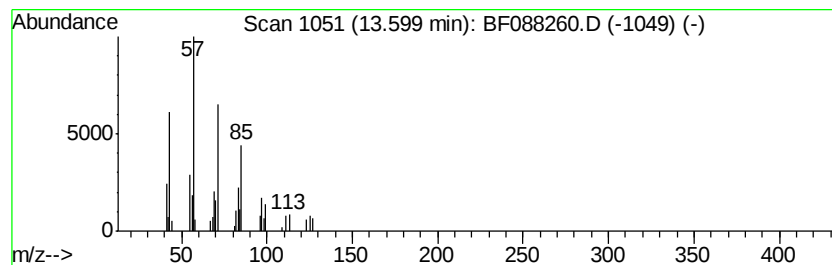
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Peak Number 5 Sulfurous acid, 2-propyl te... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.60	2.61 ng	84438	Chrysene-d12	13.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, 2-propyl tetradec...	320	C17H36O3S	1000309-12-5	90
2		Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	86
3		Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	83
4		Eicosane	282	C20H42	000112-95-8	59
5		Tridecane	184	C13H28	000629-50-5	59



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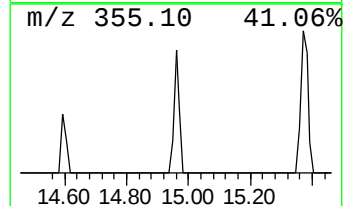
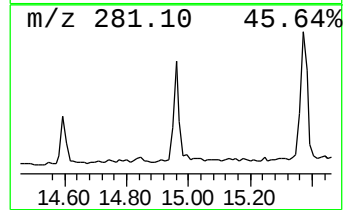
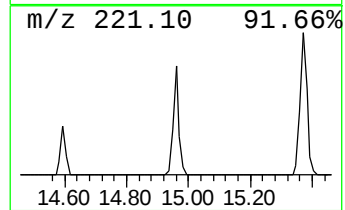
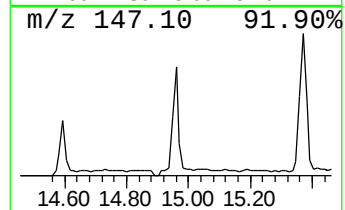
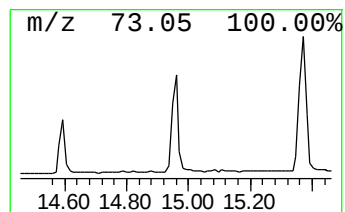
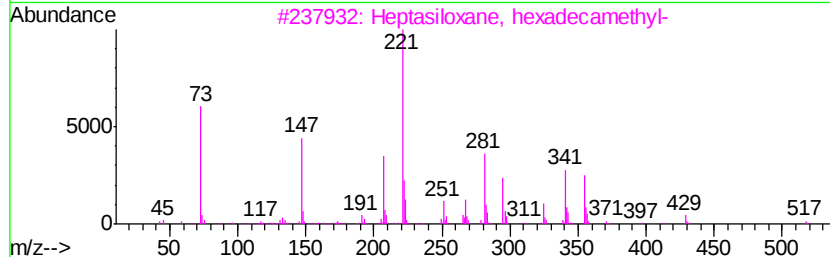
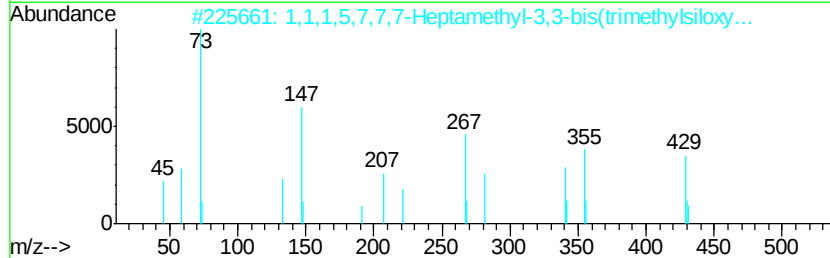
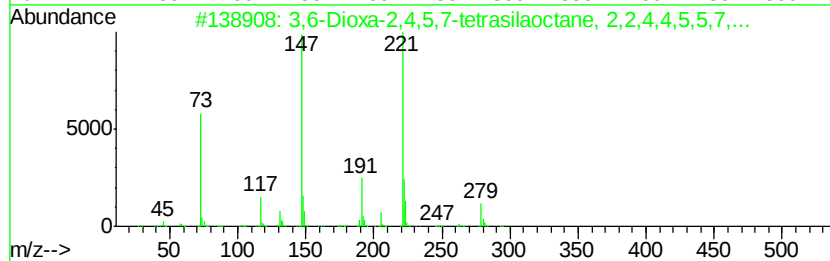
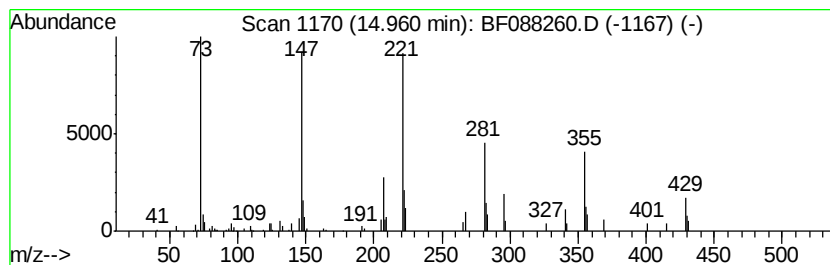
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Peak Number 7 unknown14.96 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	3.01 ng	69779	Perylene-d12	15.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H3002Si4	004342-25-0	47
2		1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H4005Si6	038147-00-1	40
3		Heptasiloxane, hexadecamethyl-	532	C16H4806Si7	000541-01-5	38
4		Mercaptoacetic acid, bis(trimeth...	236	C8H2002SSi2	006398-62-5	37
5		Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H3604Si5	003555-47-3	27



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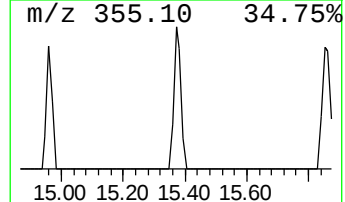
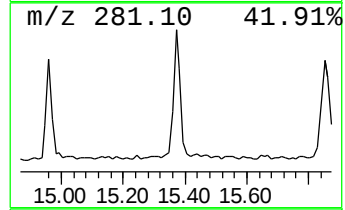
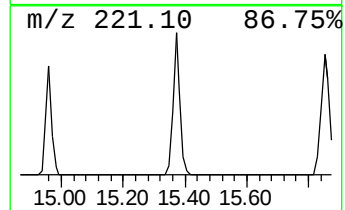
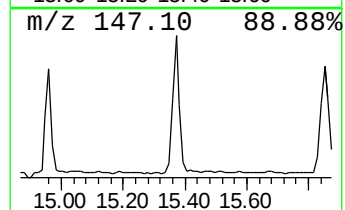
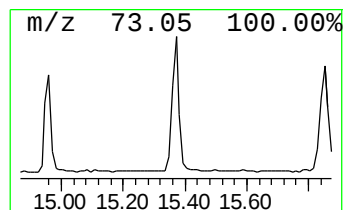
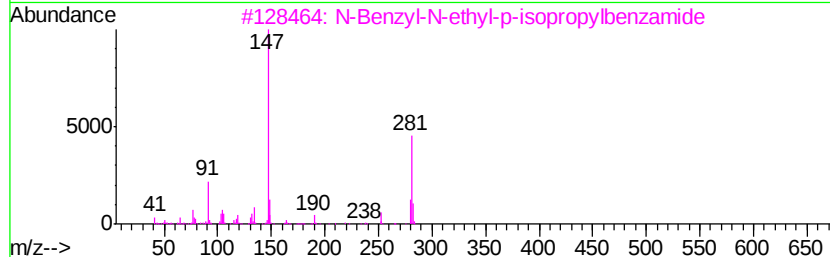
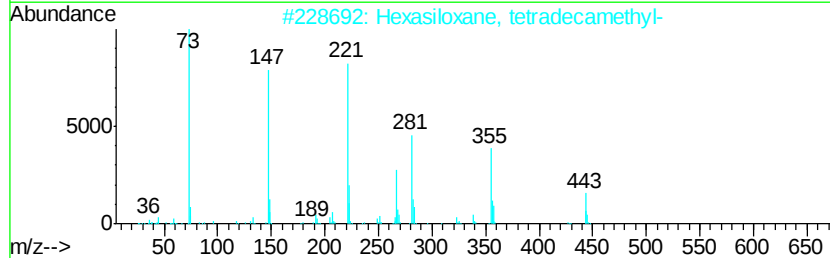
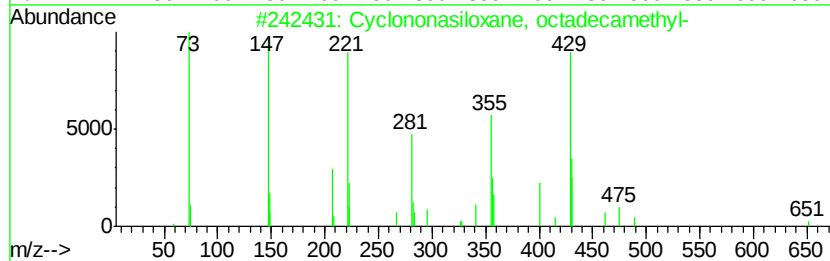
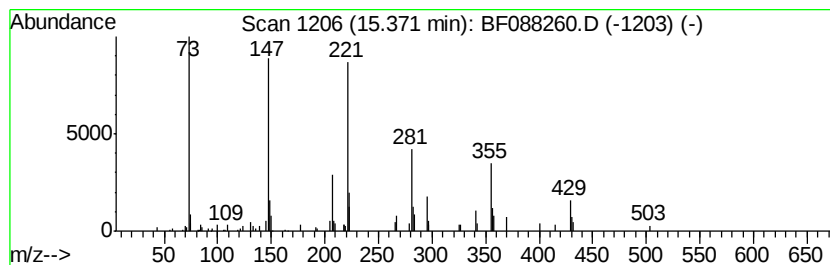
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Peak Number 8 Cyclononasiloxane, octadeca... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.37	5.40 ng	125416	Perylene-d12	15.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclononasiloxane, octadecamethyl-	666	C18H5409Si9	000556-71-8	91
2		Hexasiloxane, tetradecamethyl-	458	C14H4205Si6	000107-52-8	90
3		N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	38
4		Pentasiloxane, dodecamethyl-	384	C12H3604Si5	000141-63-9	35
5		Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H3604Si5	003555-47-3	35



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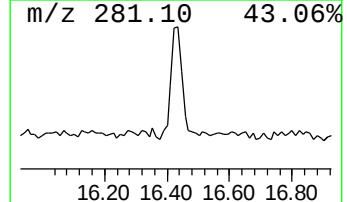
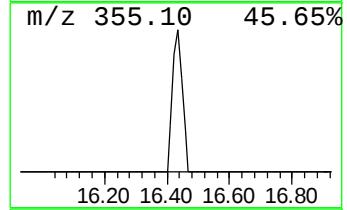
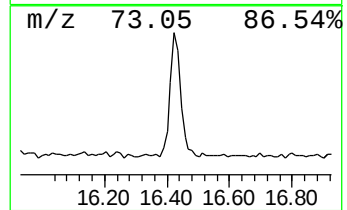
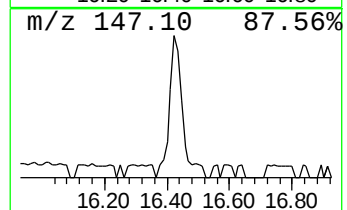
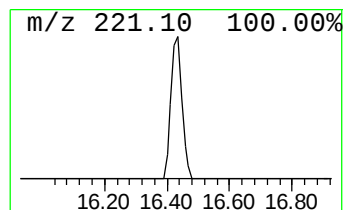
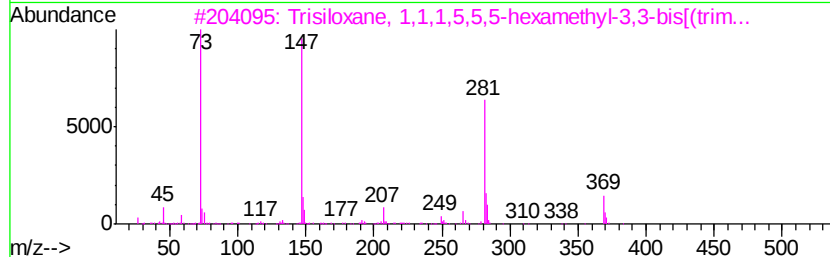
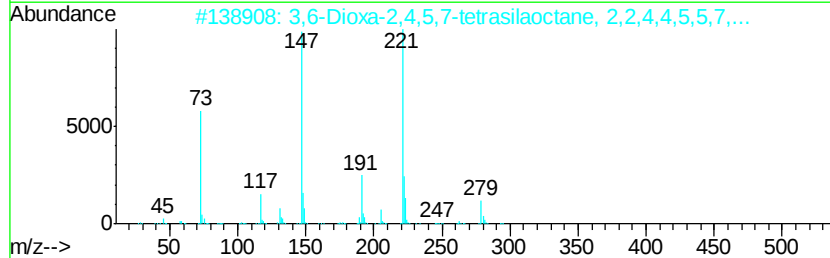
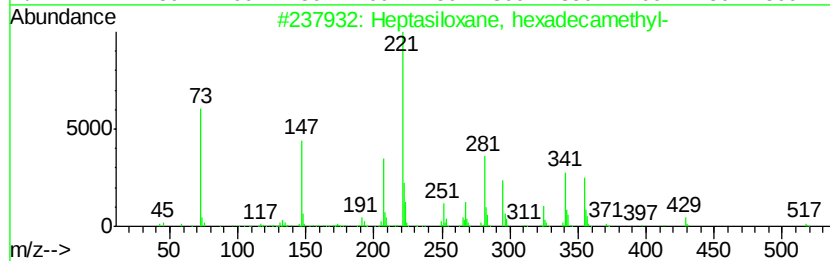
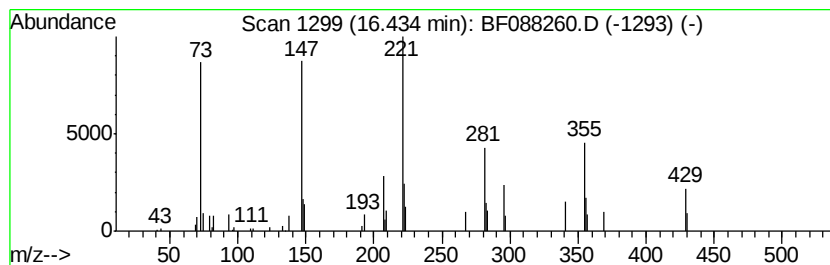
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptasiloxane, hexadecamethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.43	2.79 ng	64831	Perylene-d12	15.11

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	64
2			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	37
3			Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	27
4			3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	16
5			2,6-Dimethyl-3,4-bis(trimethylsi...	311	C15H29NO2Si2	1000079-52-1	16



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062216\
Data File : BF088260.D
Acq On : 22 Jun 2016 20:18
Operator : UM/SJ
Sample : H3678-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TDGA-MH-1617

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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...	4.73	13.2	ng	261006	1	6.60	394457	20.0
unknown6.36	6.36	77.6	ng	1531020	1	6.60	394457	20.0
Sulfurous acid, 2...	13.60	2.6	ng	84438	5	13.74	648114	20.0
unknown14.96	14.96	3.0	ng	69779	6	15.11	464256	20.0
Cyclononasiloxane...	15.37	5.4	ng	125416	6	15.11	464256	20.0
Heptasiloxane, he...	16.43	2.8	ng	64831	6	15.11	464256	20.0