

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052916\
 Data File : BF087545.D
 Acq On : 30 May 2016 11:54
 Operator : UM/SJ
 Sample : H3295-02
 Misc :
 ALS Vial : 65 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 R1-MW2-GW

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:\HPCHEM1\BNA_F\METHODS\8270-BF052316.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	4.707	270	273	291	rBV	150337	546559	13.50%	1.814%
2	5.382	330	332	355	rBV	621608	1831494	45.24%	6.080%
3	5.987	383	385	397	rBV	22102	76407	1.89%	0.254%
4	7.027	474	476	483	rBV	786969	1502718	37.12%	4.988%
5	7.130	483	485	505	rVB	1725774	3566488	88.10%	11.839%
6	7.473	514	515	527	rBV	361738	854736	21.11%	2.837%
7	7.702	533	535	552	rVV	1864974	2693704	66.54%	8.942%
8	8.388	593	595	628	rBV	1359694	2490096	61.51%	8.266%
9	9.508	691	693	708	rBV2	457120	1034052	25.54%	3.433%
10	11.279	845	848	864	rBV	3075480	4048136	100.00%	13.438%
11	12.011	909	912	918	rBV2	35340	93744	2.32%	0.311%
12	12.331	938	940	955	rBV	702148	1171317	28.93%	3.888%
13	13.165	1010	1013	1015	rVB	79281	99226	2.45%	0.329%
14	13.519	1040	1044	1046	rBV	19461	40571	1.00%	0.135%
15	13.622	1051	1053	1075	rVV	1286882	2420448	59.79%	8.035%
16	13.931	1078	1080	1086	rBV	67698	111381	2.75%	0.370%
17	14.662	1141	1144	1146	rBV2	29680	40736	1.01%	0.135%
18	14.742	1150	1151	1168	rBV	396148	1059248	26.17%	3.516%
19	15.725	1234	1237	1244	rBV2	55122	101762	2.51%	0.338%
20	16.823	1331	1333	1339	rBV2	30732	58933	1.46%	0.196%
21	16.926	1340	1342	1345	rVB	63024	68360	1.69%	0.227%
22	17.086	1354	1356	1366	rVB	2564011	3286684	81.19%	10.910%
23	18.354	1463	1467	1475	rBV2	42007	149566	3.69%	0.496%
24	18.469	1475	1477	1492	rVV	292305	726841	17.95%	2.413%
25	19.600	1574	1576	1580	rVB	30302	42563	1.05%	0.141%
26	20.034	1611	1614	1617	rBV	70506	111319	2.75%	0.370%
27	20.160	1623	1625	1646	rBV	188212	661250	16.33%	2.195%
28	20.434	1646	1649	1655	rVB	129833	191433	4.73%	0.635%
29	20.880	1685	1688	1697	rVB	128807	262210	6.48%	0.870%
30	21.406	1727	1734	1739	rBV2	117476	262258	6.48%	0.871%
31	22.035	1784	1789	1796	rVB	83592	220689	5.45%	0.733%
32	22.800	1850	1856	1863	rVB	51969	172822	4.27%	0.574%
33	23.726	1931	1937	1944	rBV3	31936	127050	3.14%	0.422%

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Misc :
ALS Vial : 65 Sample Multiplier: 1

Instrument :
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ClientSampleId :
R1-MW2-GW

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-BF052316.M
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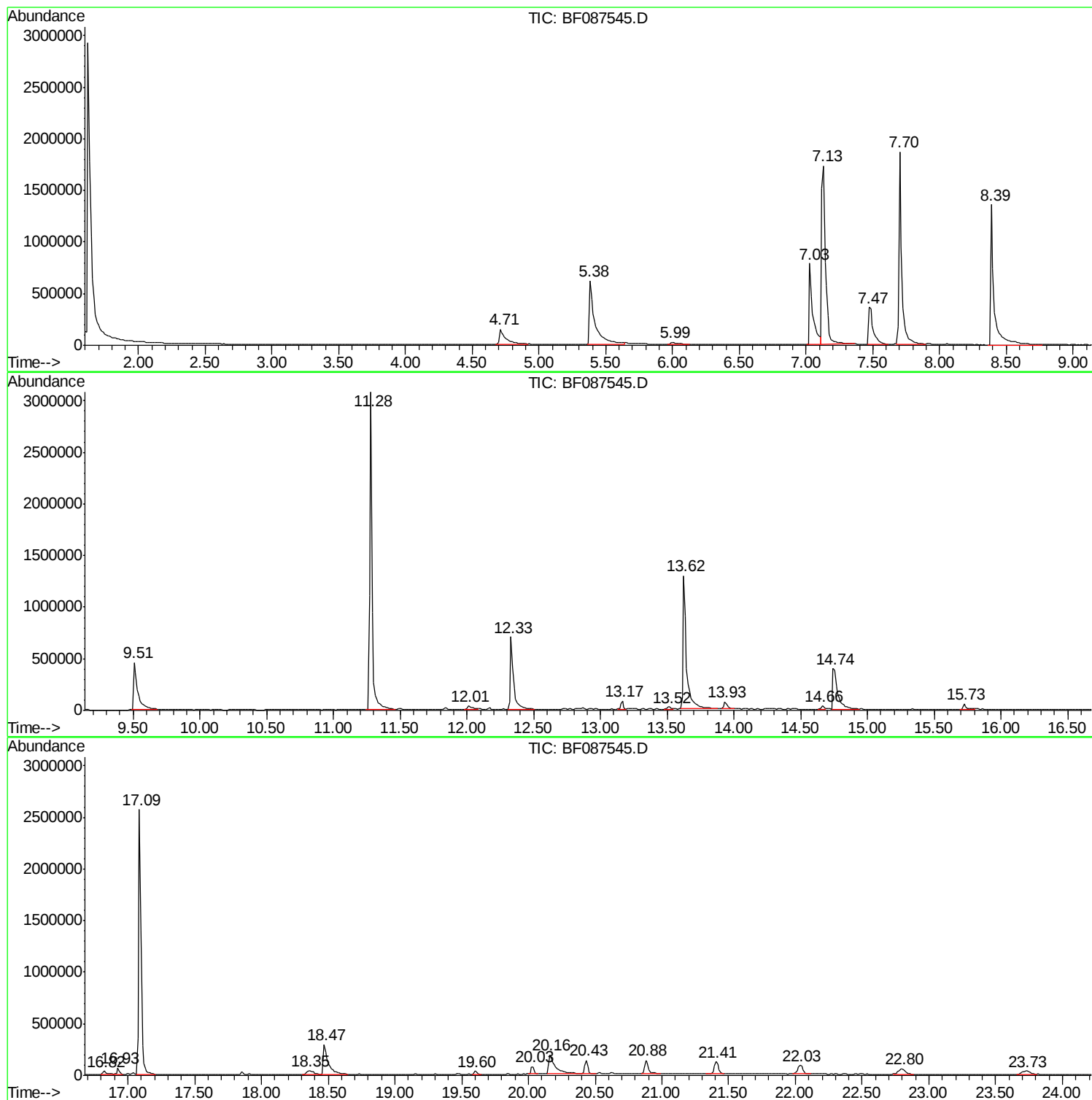
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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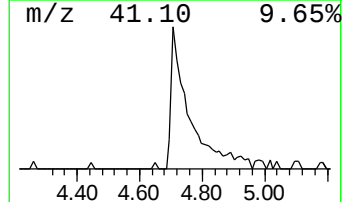
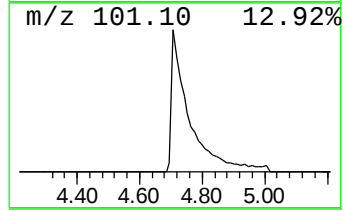
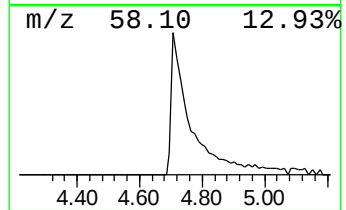
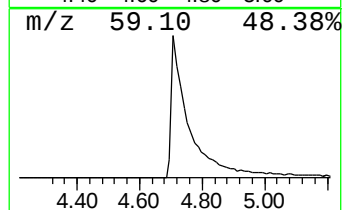
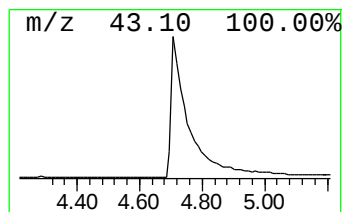
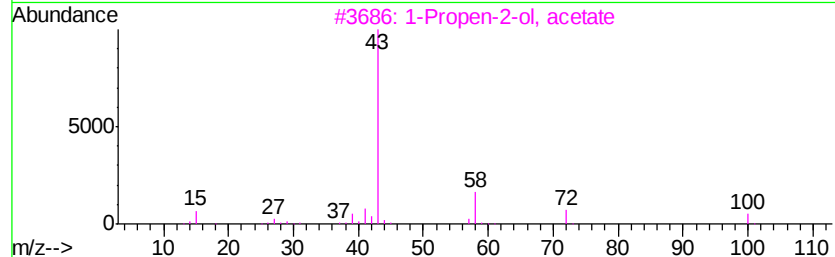
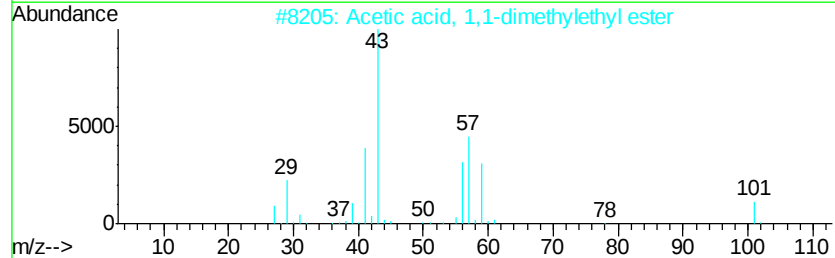
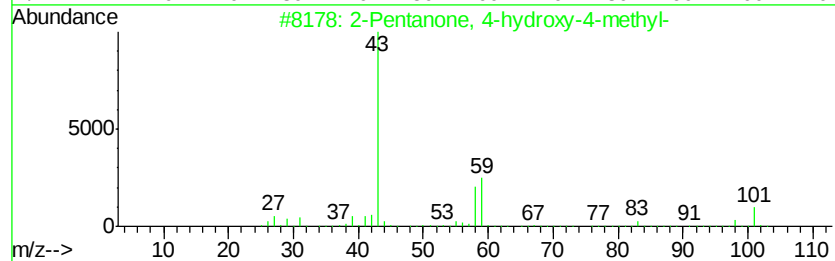
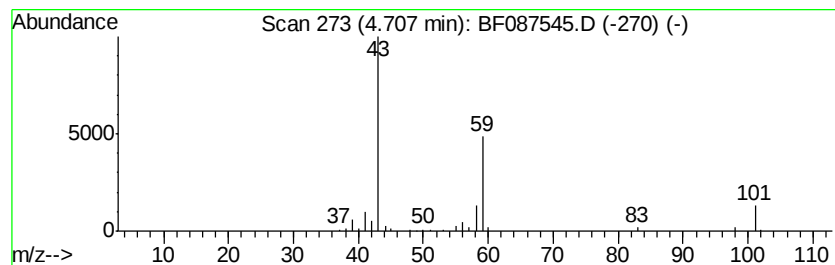
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.71	12.79 ng	546559	1,4-Dichlorobenzene-d4	7.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		Diacetamide	101	C4H7NO2	000625-77-4	9
5		4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9



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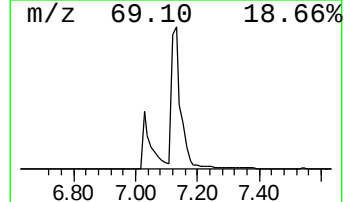
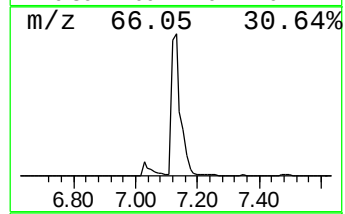
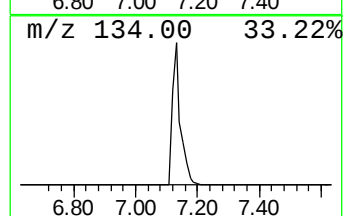
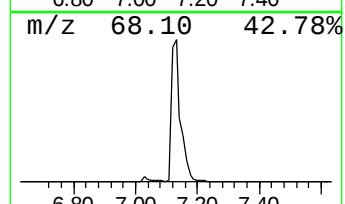
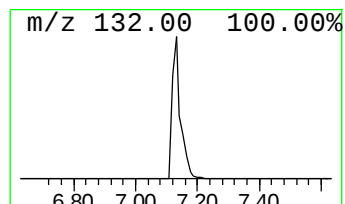
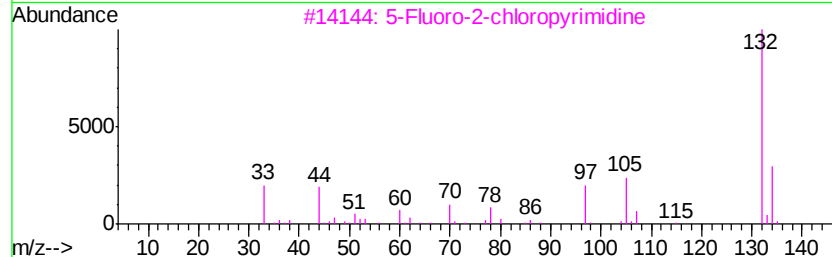
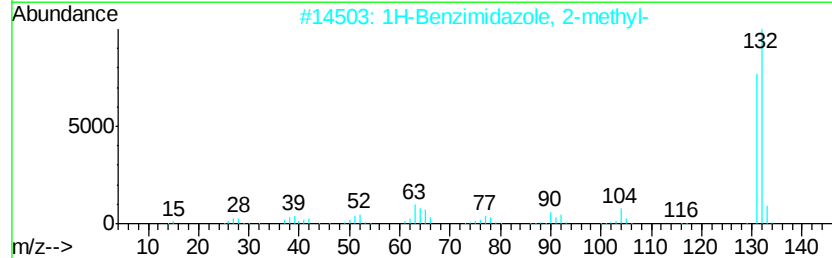
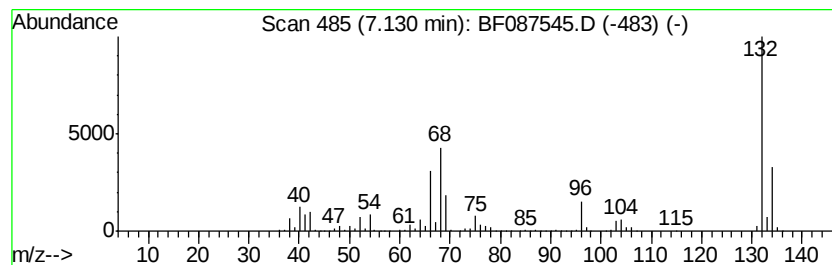
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TIC Library : C:\Database\NIST11.L
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Peak Number 2 unknown7.13 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.13	83.45 ng	3566490	1,4-Dichlorobenzene-d4	7.48

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-			132	C8H8N2	000615-15-6	22
3	5-Fluoro-2-chloropyrimidine			132	C4H2ClFN2	062802-42-0	12
4	(5-Methyl-2-pyridyl)acetonitrile			132	C8H8N2	1000241-93-9	10
5	Bicyclo[4.2.0]octa-1,3,5-triene, ...			132	C10H12	028749-81-7	9



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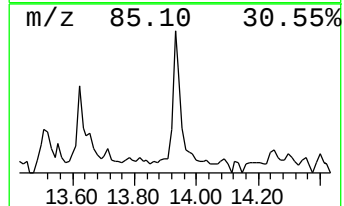
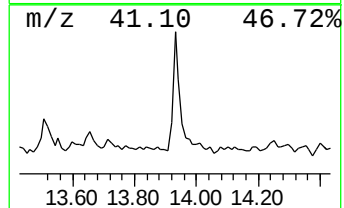
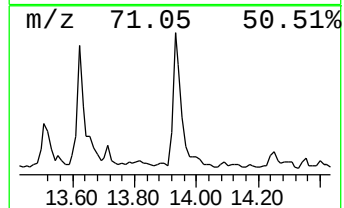
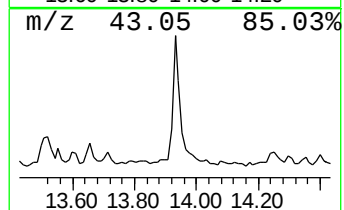
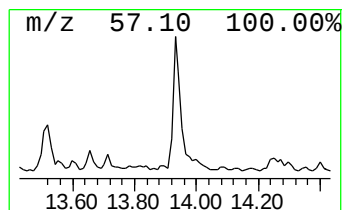
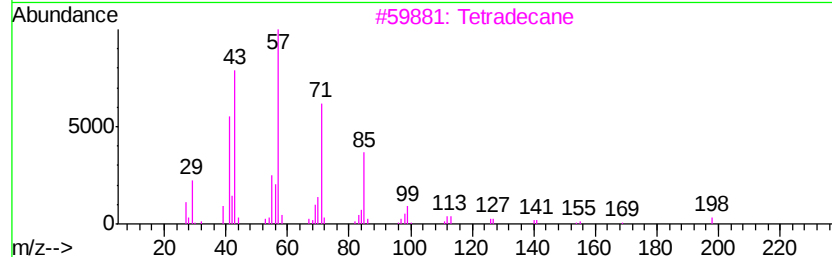
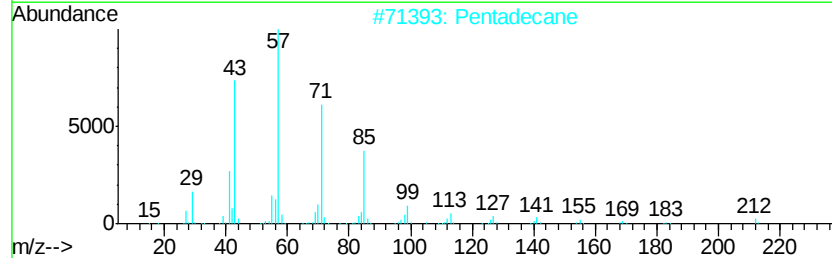
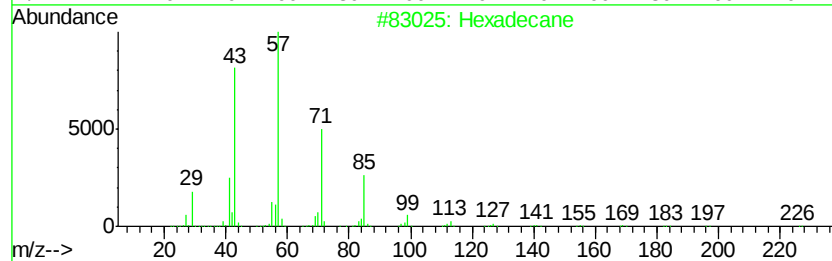
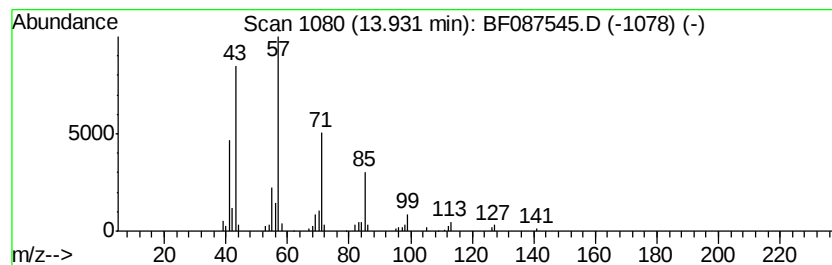
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TIC Library : C:\Database\NIST11.L
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Peak Number 4 Hexadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	2.10 ng	111381	Phenanthrene-d10	14.75

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	91
2	Pentadecane		212	C15H32	000629-62-9	90
3	Tetradecane		198	C14H30	000629-59-4	86
4	Tridecane		184	C13H28	000629-50-5	80
5	1-Iodo-2-methylundecane		296	C12H25I	073105-67-6	80



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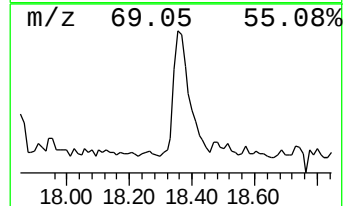
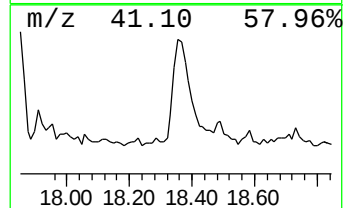
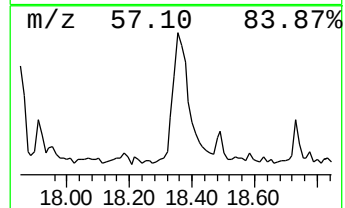
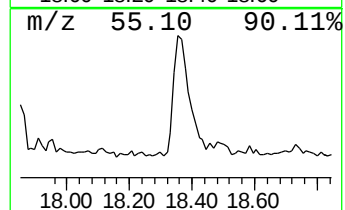
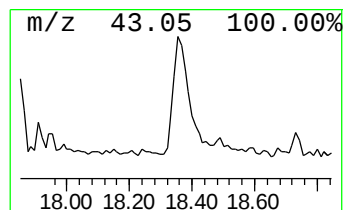
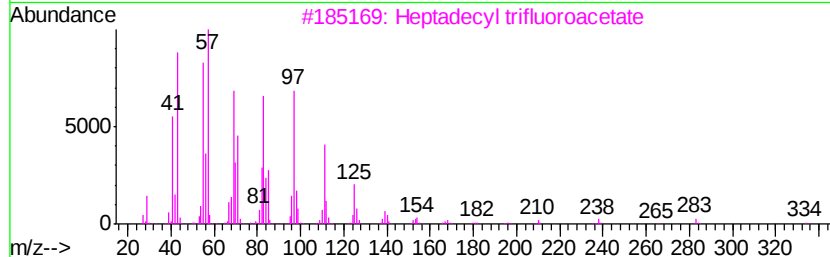
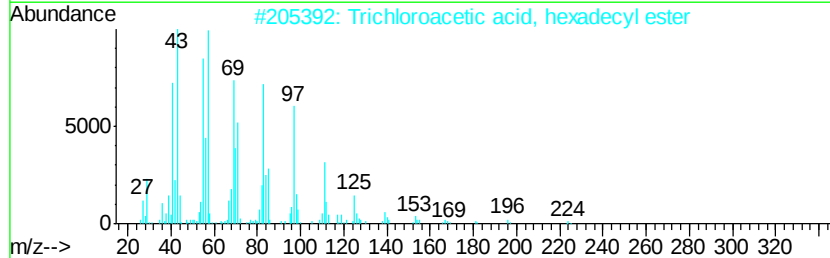
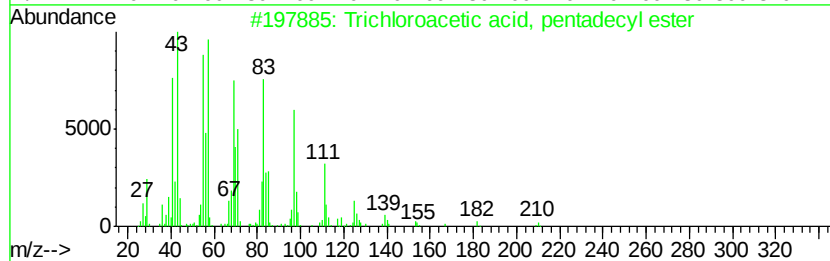
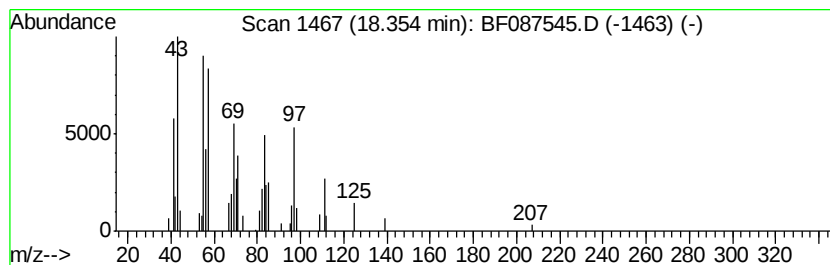
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Trichloroacetic acid, penta... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.35	4.12 ng	149566	Chrysene-d12	18.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
4		11-Tricosene	322	C23H46	052078-56-5	91
5		1-Docosene	308	C22H44	001599-67-3	90



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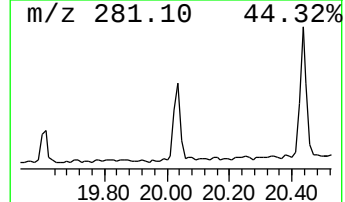
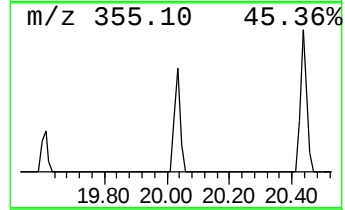
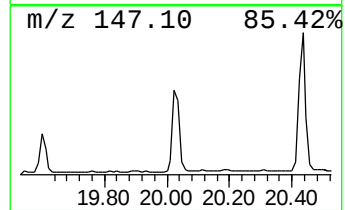
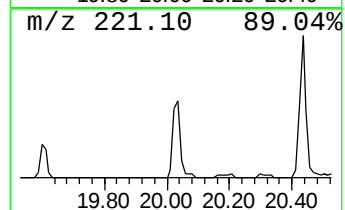
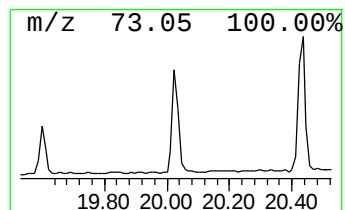
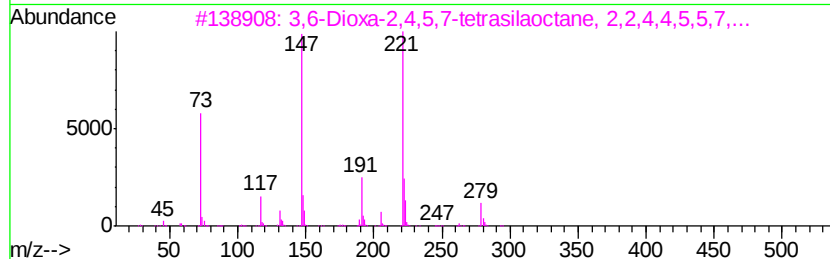
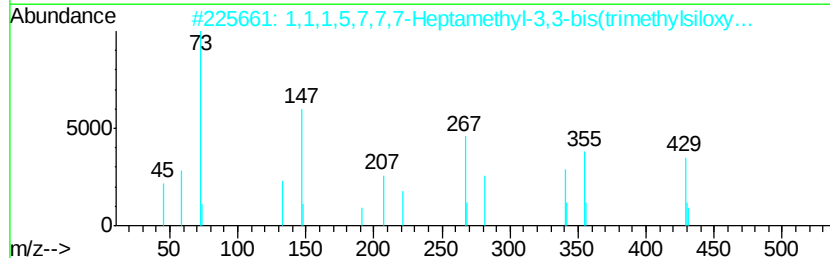
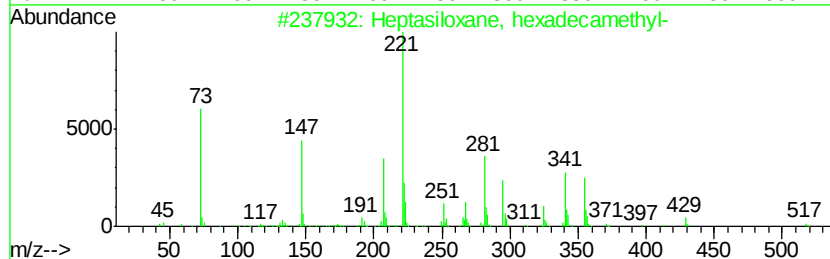
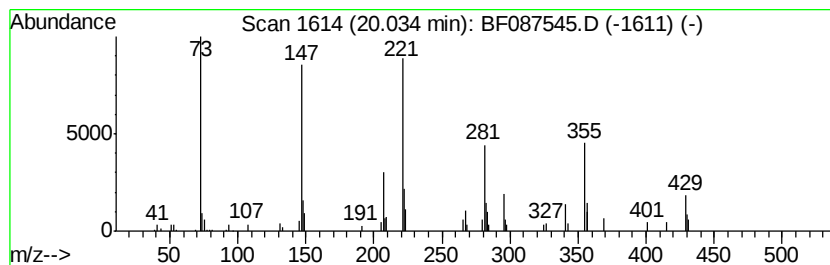
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Peak Number 6 unknown20.03 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.03	3.37 ng	111319	Perylene-d12	20.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	43
2		1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	40
3		3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	38
4		Mercaptoacetic acid, bis(trimeth...	236	C8H20O2SSi2	006398-62-5	38
5		3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	37



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R1-MW2-GW

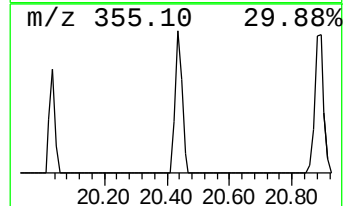
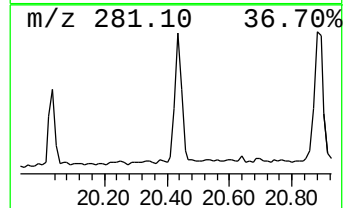
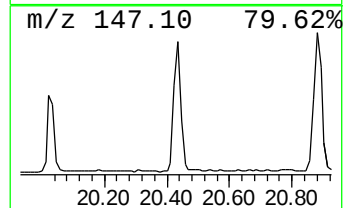
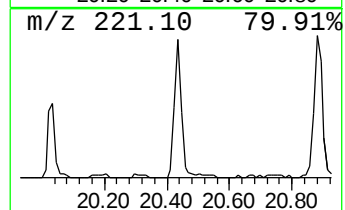
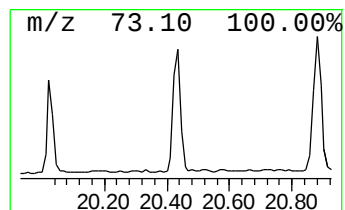
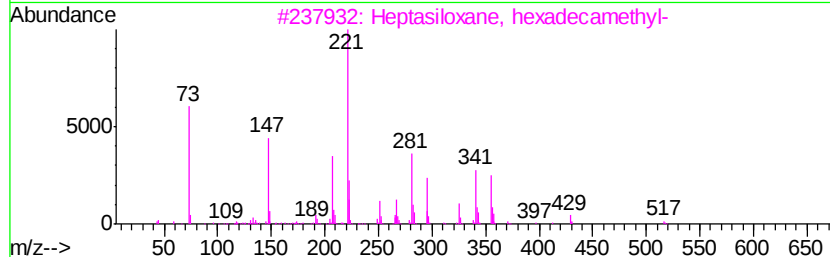
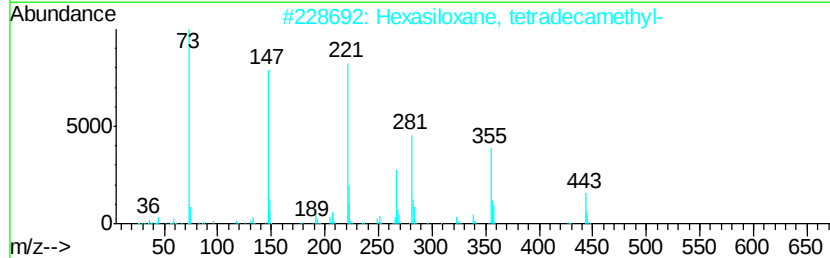
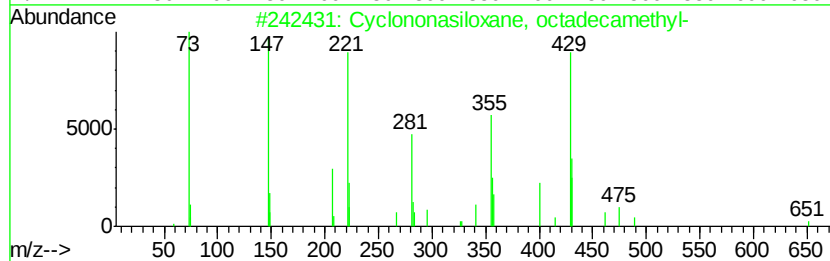
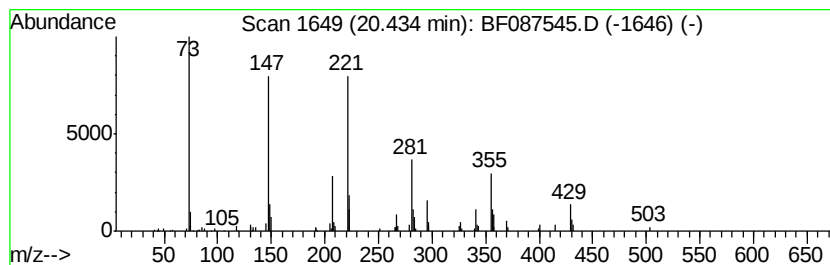
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cyclononasiloxane, octadeca... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.43	5.79 ng	191433	Perylene-d12	20.16

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H5409Si9	000556-71-8	91
2			Hexasiloxane, tetradecamethyl-	458	C14H4205Si6	000107-52-8	83
3			Heptasiloxane, hexadecamethyl-	532	C16H4806Si7	000541-01-5	78
4			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H3002Si4	004342-25-0	40
5			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	30



Data Path : Z:\HPCHEM1\BNA F\DATA\BF052916\
Data File : BF087545.D
Acq On : 30 May 2016 11:54
Operator : UM/SJ
Sample : H3295-02
Misc :
ALS Vial : 65 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
R1-MW2-GW

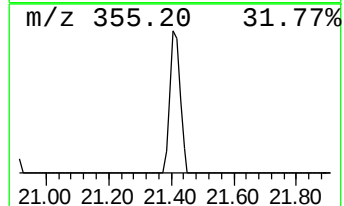
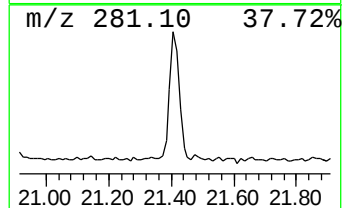
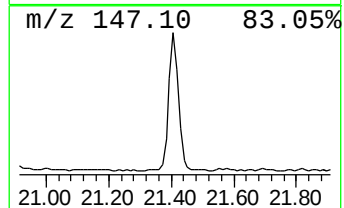
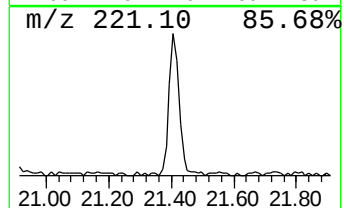
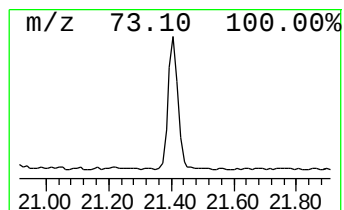
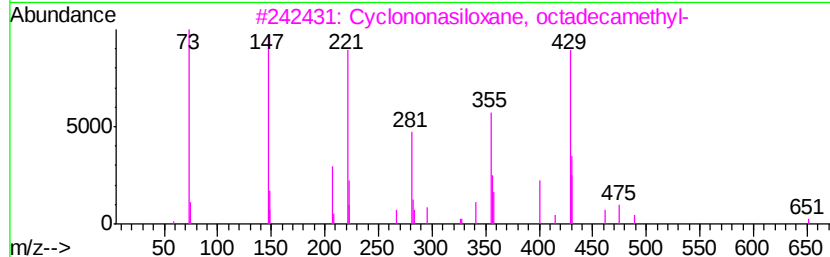
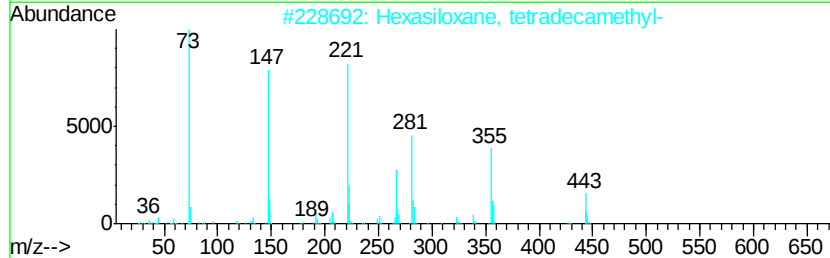
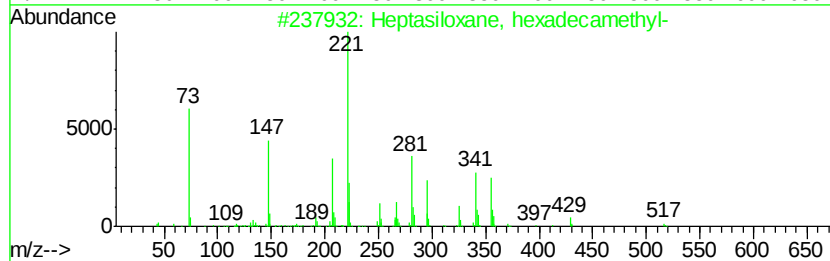
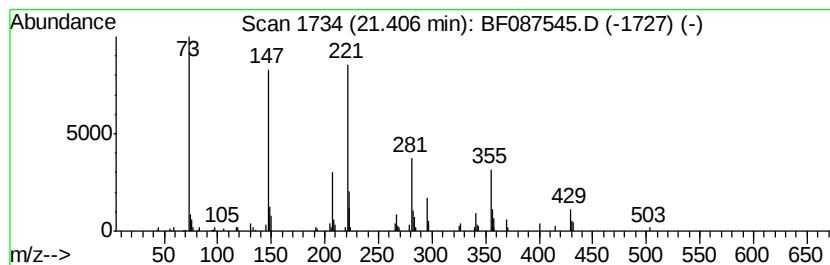
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptasiloxane, hexadecamethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.41	7.93 ng	262258	Perylene-d12	20.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	90
2	Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	80
3	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	78
4	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	53
5	Dithioerythritol, 0,0',S,S'-tetr...	442	C16H42O2S2Si4	1000079-30-7	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052916\
Data File : BF087545.D
Acq On : 30 May 2016 11:54
Operator : UM/SJ
Sample : H3295-02
Misc :
ALS Vial : 65 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
R1-MW2-GW

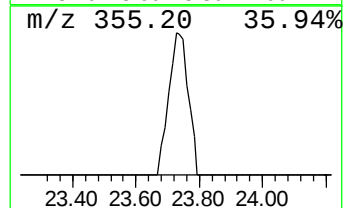
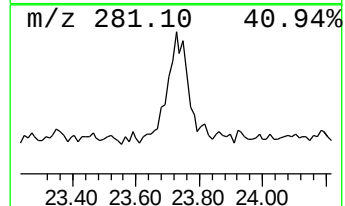
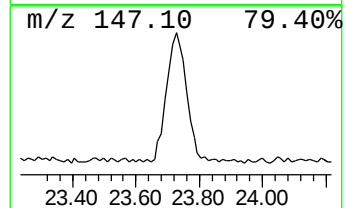
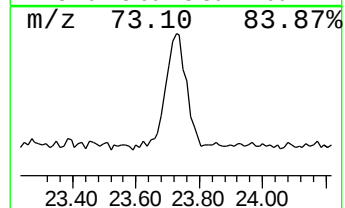
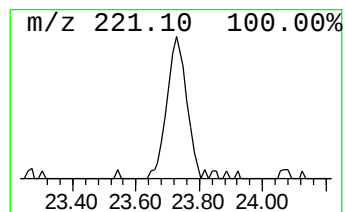
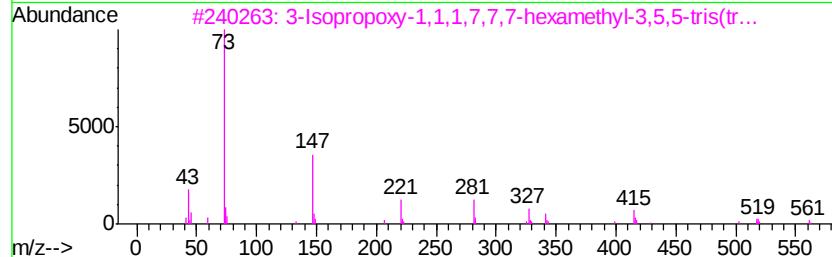
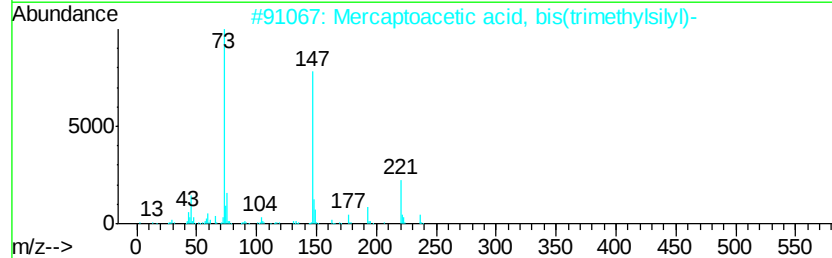
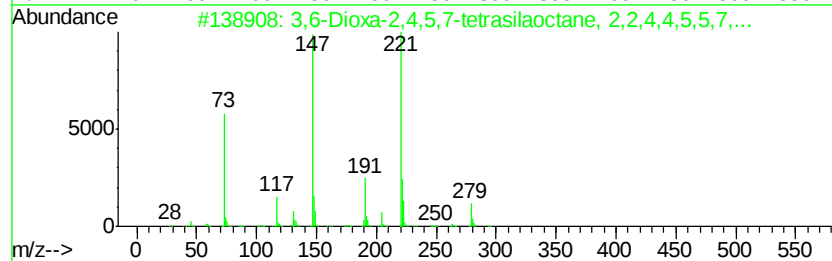
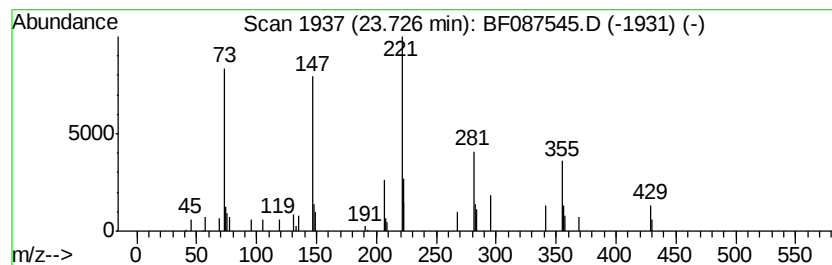
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 3,6-Dioxa-2,4,5,7-tetrasilaoctan... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.73	3.84 ng	127050	Perylene-d12	20.16

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	50
2			Mercaptoacetic acid, bis(trimeth...	236	C8H20O2SSi2	006398-62-5	38
3			3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	37
4			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	27
5			Trisiloxane, octamethyl-	236	C8H24O2Si3	000107-51-7	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052916\
Data File : BF087545.D
Acq On : 30 May 2016 11:54
Operator : UM/SJ
Sample : H3295-02
Misc :
ALS Vial : 65 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
R1-MW2-GW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.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...	4.71	12.8	ng	546559	1	7.48	854736	20.0
unknown7.13	7.13	83.5	ng	3566490	1	7.48	854736	20.0
Hexadecane	13.93	2.1	ng	111381	4	14.75	1059250	20.0
Trichloroacetic a...	18.35	4.1	ng	149566	5	18.47	726841	20.0
unknown20.03	20.03	3.4	ng	111319	6	20.16	661250	20.0
Cyclononasiloxane...	20.43	5.8	ng	191433	6	20.16	661250	20.0
Heptasiloxane, he...	21.41	7.9	ng	262258	6	20.16	661250	20.0
3,6-Dioxa-2,4,5,7...	23.73	3.8	ng	127050	6	20.16	661250	20.0