

Data Path : Z:\HPCHEM1\BNA F\DATA\BF082616\
 Data File : BF089914.D
 Acq On : 26 Aug 2016 18:17
 Operator : UM/SJ
 Sample : PB93122BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB93122BL

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-BF081916.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	1.644	3	5	13	rBV	1465895	3653356	23.39%	4.693%
2	1.758	13	15	72	rVB	5282575	15620849	100.00%	20.064%
3	4.787	277	280	288	rBV	842739	1229227	7.87%	1.579%
4	5.233	316	319	321	rBV	5004233	5518334	35.33%	7.088%
5	6.296	408	412	414	rBV	3763419	5717147	36.60%	7.343%
6	6.410	419	422	425	rBV	4537222	5556824	35.57%	7.137%
7	6.650	440	443	445	rBV	1688430	1615639	10.34%	2.075%
8	6.799	454	456	459	rBV	3489138	4638255	29.69%	5.958%
9	7.210	489	492	495	rBV	2754549	3293517	21.08%	4.230%
10	7.930	552	555	558	rBV	2352019	2121966	13.58%	2.726%
11	9.016	647	650	652	rBV	6525406	7142377	45.72%	9.174%
12	9.679	705	708	710	rBV	2884910	2513943	16.09%	3.229%
13	10.468	773	777	779	rBV	3035145	4104668	26.28%	5.272%
14	11.154	834	837	839	rBV	2978062	2640132	16.90%	3.391%
15	12.742	973	976	978	rBV	5940487	6370513	40.78%	8.183%
16	13.771	1063	1066	1068	rBV	2670621	2424925	15.52%	3.115%
17	15.040	1174	1177	1181	rVB	130853	180553	1.16%	0.232%
18	15.120	1181	1184	1187	rBV	1481032	1943091	12.44%	2.496%
19	15.474	1211	1215	1220	rBV	180425	301055	1.93%	0.387%
20	15.977	1255	1259	1266	rBV	195446	408031	2.61%	0.524%
21	16.583	1307	1312	1322	rVB	142028	377090	2.41%	0.484%
22	17.314	1370	1376	1387	rBV	81944	289896	1.86%	0.372%
23	18.229	1449	1456	1466	rBV2	44946	192606	1.23%	0.247%

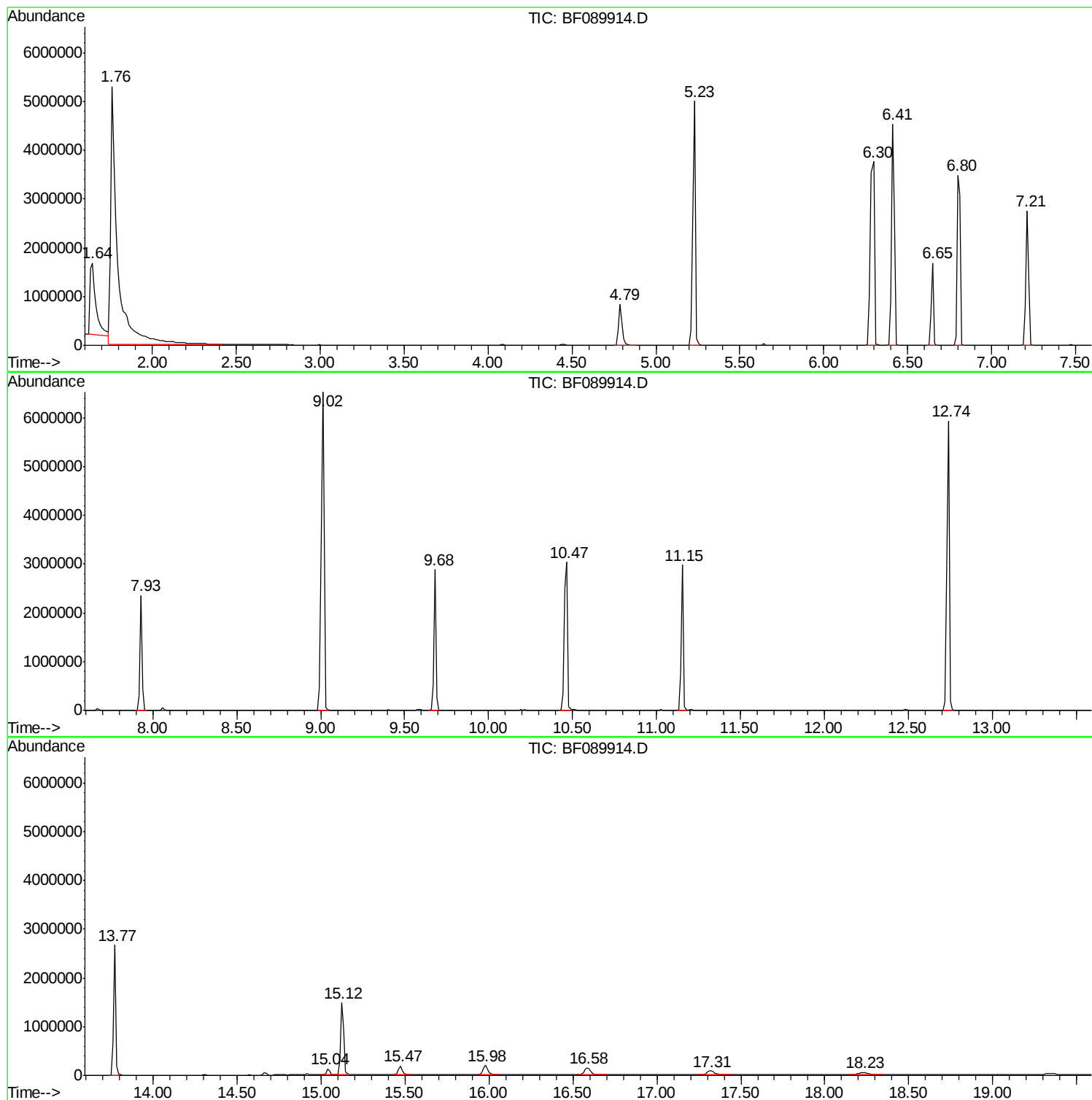
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Acq On : 26 Aug 2016 18:17
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Sample : PB93122BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
PB93122BL

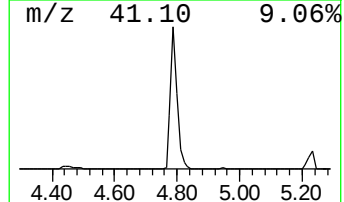
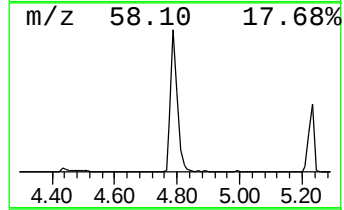
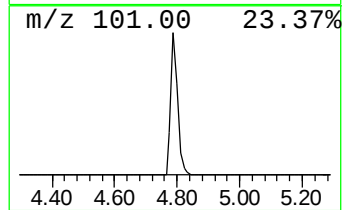
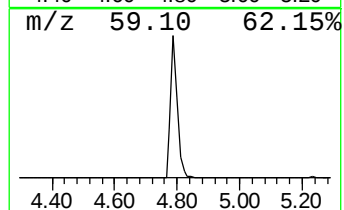
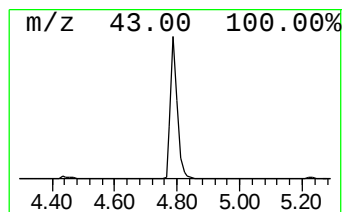
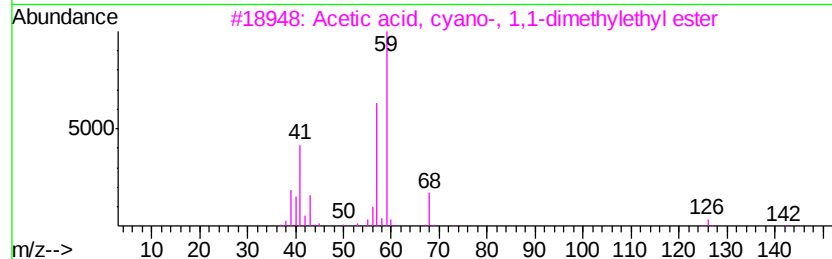
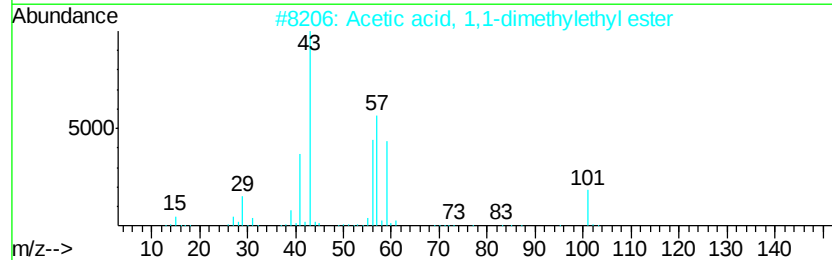
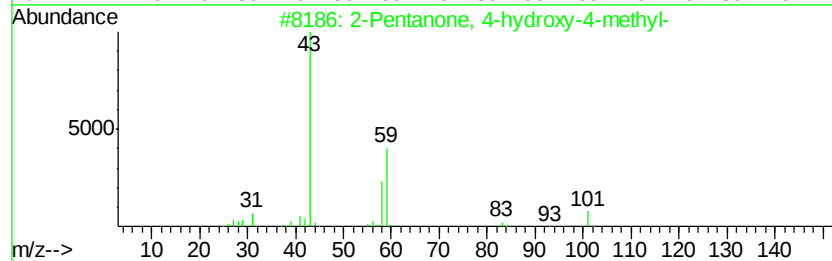
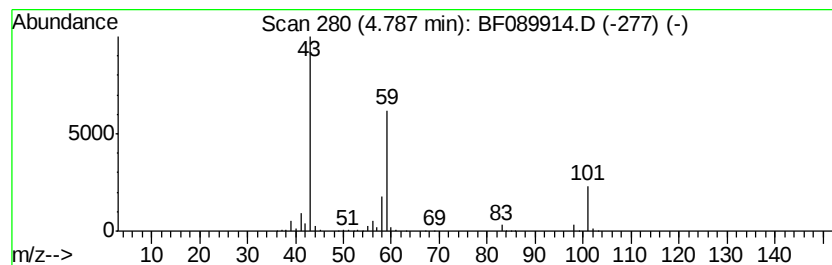
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.79	15.22 ng	1229230	1,4-Dichlorobenzene-d4	6.65

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-			116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...			116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethyl...			141	C7H11NO2	001116-98-9	23
4	5-Hexen-2-one			98	C6H10O	000109-49-9	9
5	Butane, 1-ethoxy-			102	C6H14O	000628-81-9	9



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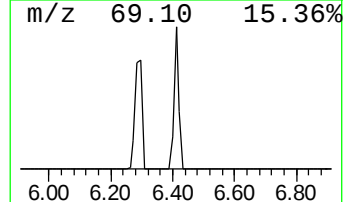
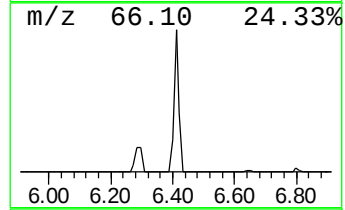
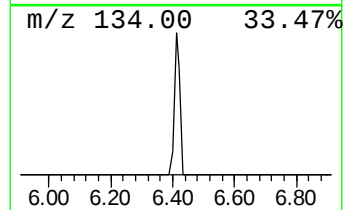
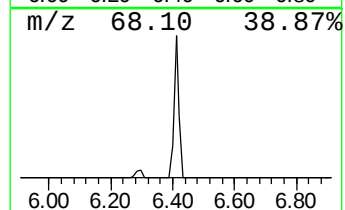
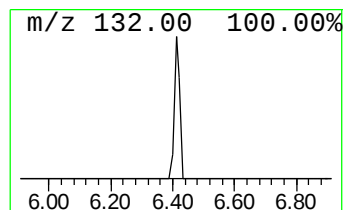
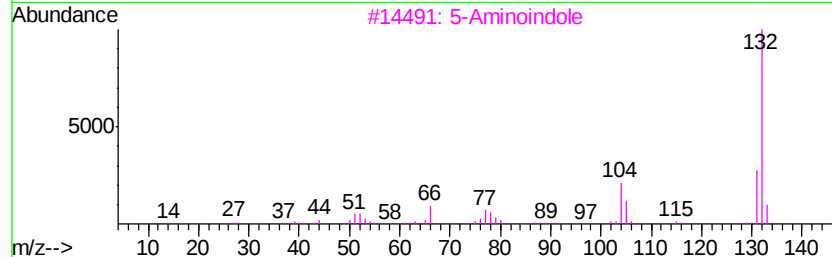
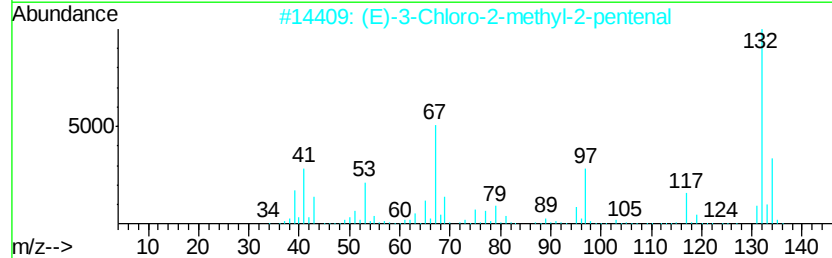
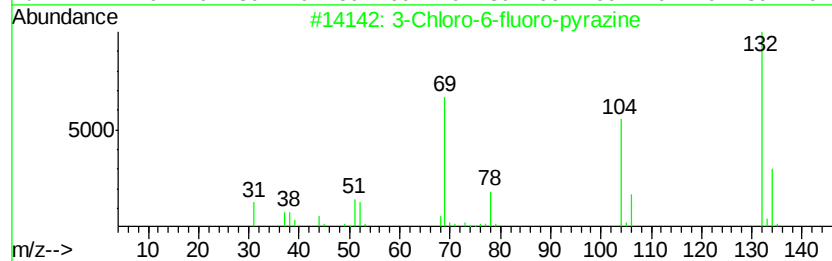
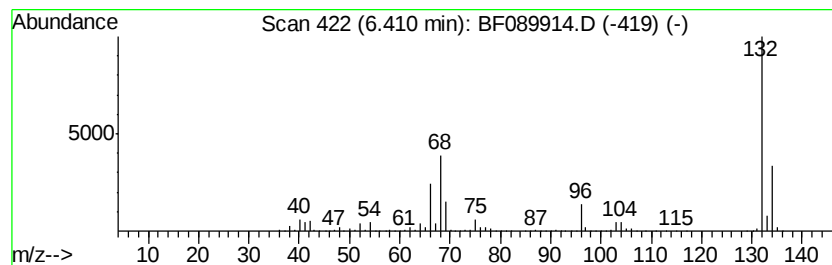
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.41 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.41	68.79 ng	5556820	1,4-Dichlorobenzene-d4	6.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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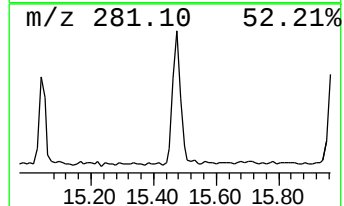
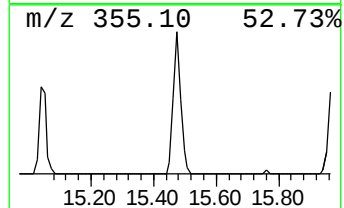
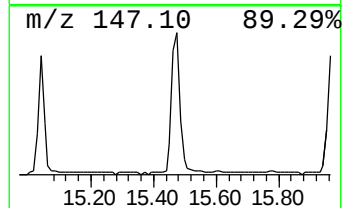
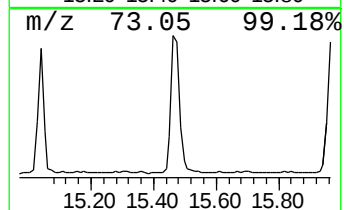
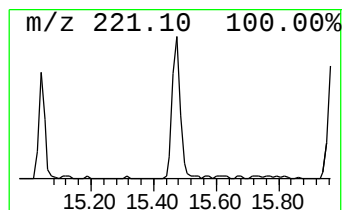
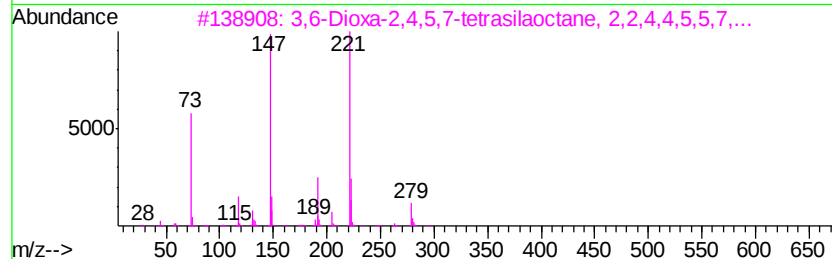
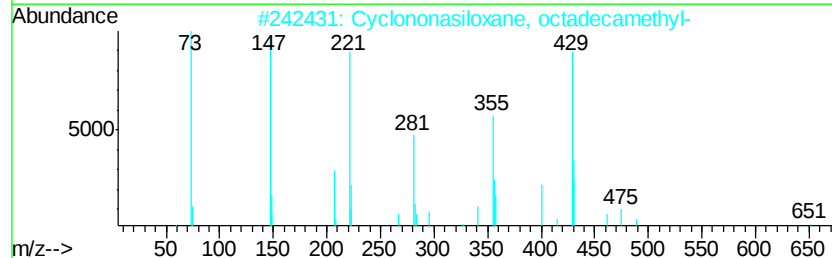
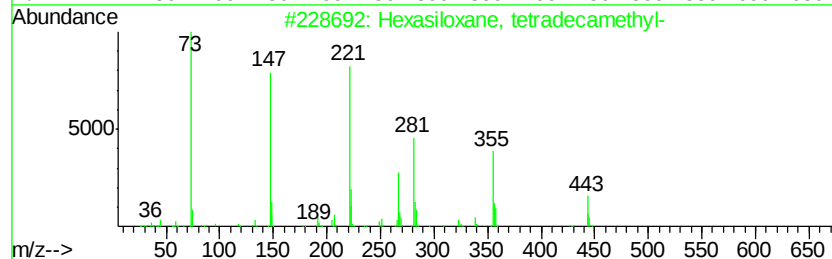
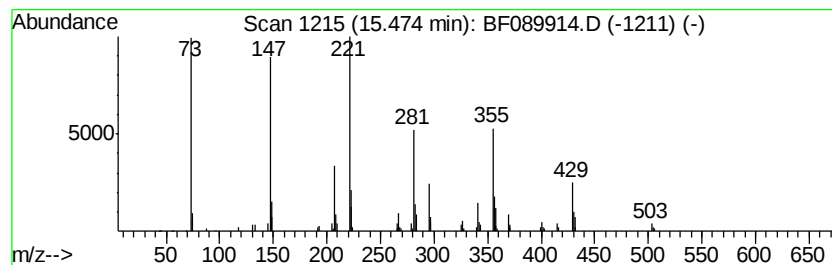
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Peak Number 6 Hexasiloxane, tetradecamethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.47	3.10 ng	301055	Perylene-d12	15.12

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	81
2			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	72
3			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	43
4			Mercaptoacetic acid, bis(trimeth...	236	C8H20O2SSi2	006398-62-5	37
5			Dithioerythritol, 0,0',S,S'-tetr...	442	C16H42O2S2Si4	1000079-30-7	27



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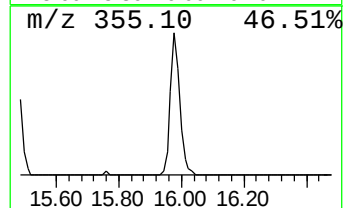
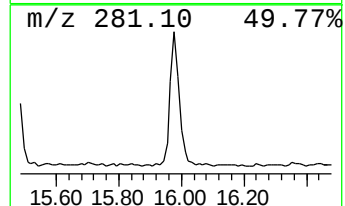
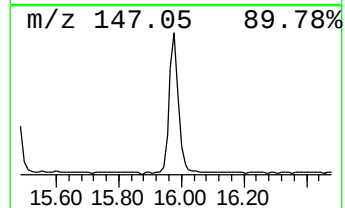
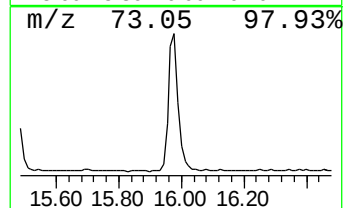
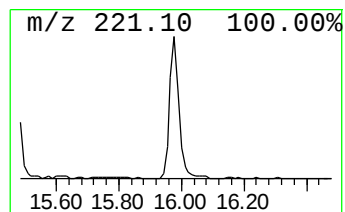
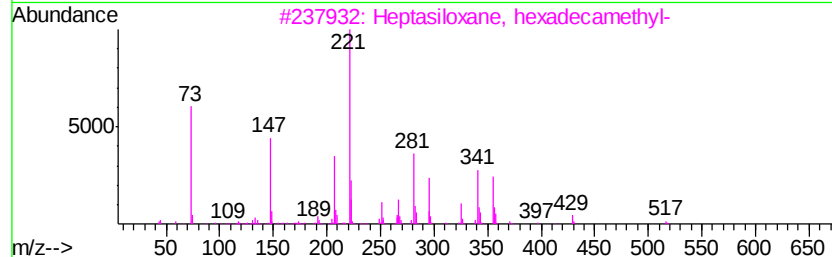
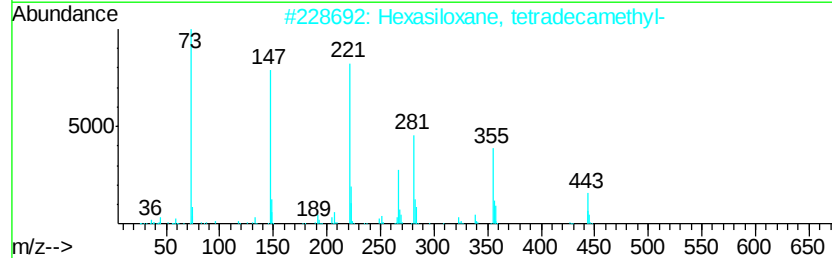
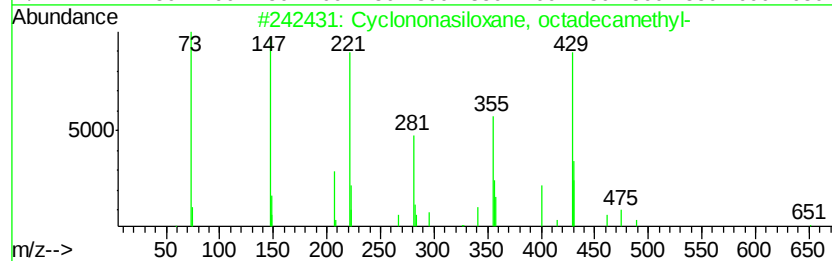
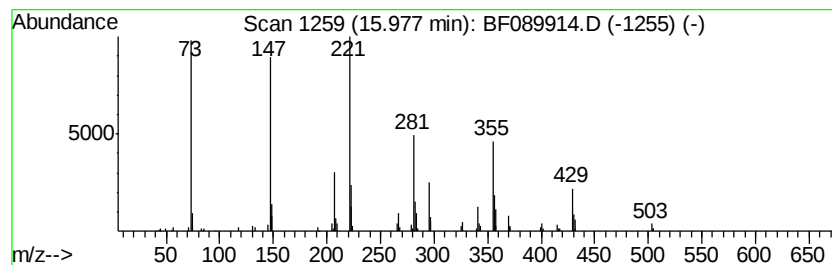
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Peak Number 7 Cyclononasiloxane, octadeca... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.98	4.20 ng	408031	Perylene-d12	15.12

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	83
2		Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	64
3		Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	50
4		3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	37
5		1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	37



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.79	15.2	ng	1229230	1	6.65	1615640	20.0
unknown6.41	6.41	68.8	ng	5556820	1	6.65	1615640	20.0
Hexasiloxane, tet...	15.47	3.1	ng	301055	6	15.12	1943090	20.0
Cyclononasiloxane...	15.98	4.2	ng	408031	6	15.12	1943090	20.0