

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051717\
 Data File : BF095213.D
 Acq On : 18 May 2017 8:07
 Operator : SJ/MA
 Sample : I3192-01
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 051617-01

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-BF050217.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	5.125	538	542	560	rBV	139229	334001	14.10%	1.834%
2	5.742	643	647	674	rBV	943429	2033401	85.85%	11.162%
3	7.313	910	914	930	rBV	1266370	2013632	85.02%	11.054%
4	7.436	930	935	954	rVB	1568721	2368478	100.00%	13.002%
5	7.772	988	992	1006	rBV	392380	474791	20.05%	2.606%
6	8.007	1027	1032	1045	rBV	1333043	1622290	68.50%	8.906%
7	8.666	1140	1144	1161	rBV	704304	1107786	46.77%	6.081%
8	9.789	1330	1335	1355	rBV	397942	614113	25.93%	3.371%
9	10.848	1510	1515	1520	rBV	81049	100122	4.23%	0.550%
10	11.560	1631	1636	1655	rBV	1726174	2311043	97.58%	12.687%
11	12.254	1750	1754	1766	rBV	192714	313339	13.23%	1.720%
12	12.348	1766	1770	1774	rVB	35061	42224	1.78%	0.232%
13	12.618	1812	1816	1832	rBV2	379399	617224	26.06%	3.388%
14	13.454	1954	1958	1963	rVB	26456	29695	1.25%	0.163%
15	13.918	2032	2037	2051	rBV	573884	947203	39.99%	5.200%
16	14.224	2086	2089	2093	rBV	32421	45312	1.91%	0.249%
17	14.960	2210	2214	2218	rBV	25337	33324	1.41%	0.183%
18	15.024	2218	2225	2238	rVV2	296359	489776	20.68%	2.689%
19	15.618	2322	2326	2331	rBV	22442	27022	1.14%	0.148%
20	15.983	2382	2388	2399	rBV5	13661	39085	1.65%	0.215%
21	16.818	2526	2530	2536	rBV	17962	24918	1.05%	0.137%
22	17.118	2577	2581	2590	rVB	22786	29669	1.25%	0.163%
23	17.342	2614	2619	2632	rBV	1416013	1651944	69.75%	9.068%
24	18.695	2845	2849	2863	rBV	332949	473481	19.99%	2.599%
25	19.812	3034	3039	3045	rVB	80289	89214	3.77%	0.490%
26	20.100	3083	3088	3094	rVB6	14336	24327	1.03%	0.134%
27	20.371	3130	3134	3144	rBV	243206	359118	15.16%	1.971%

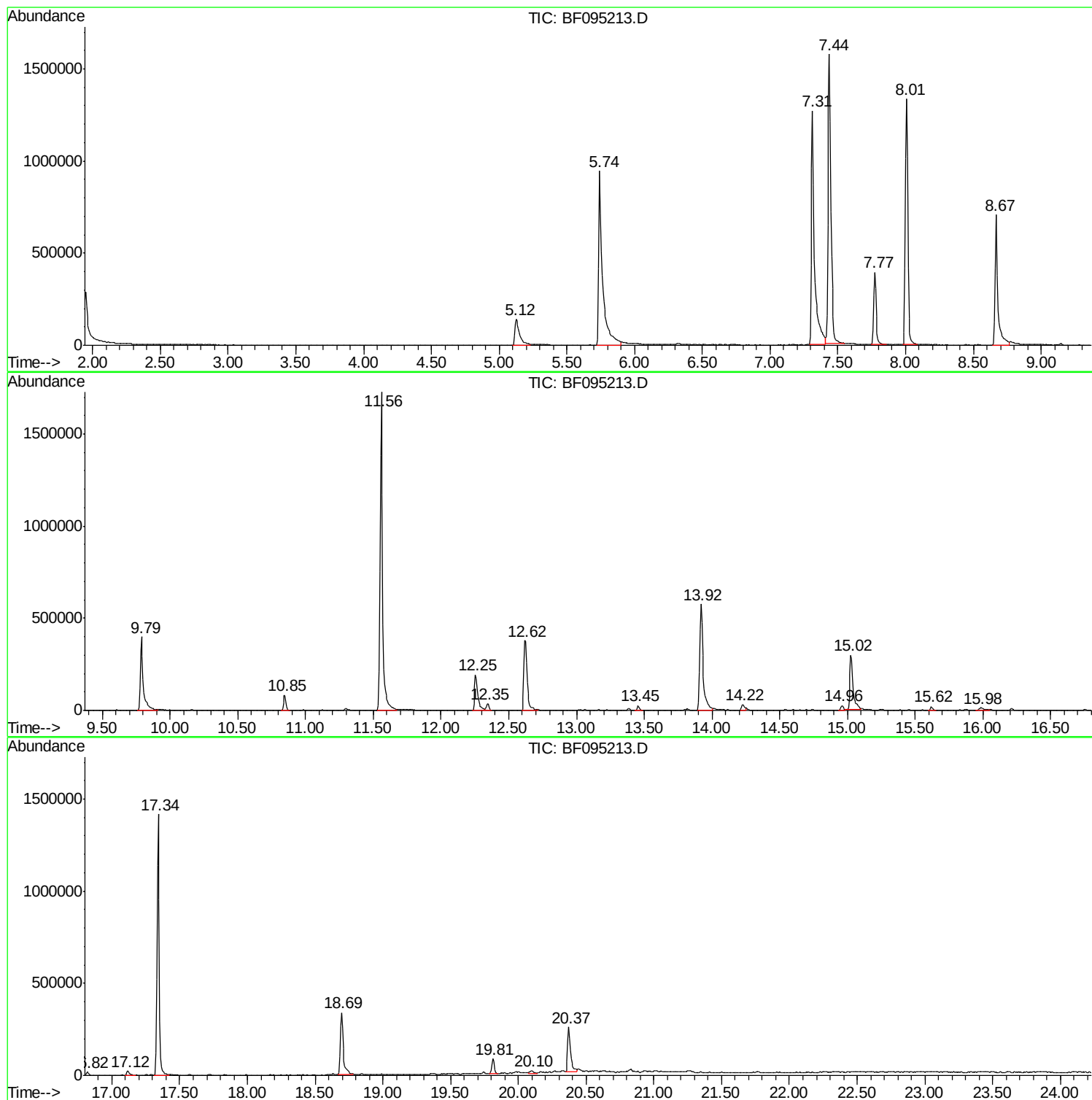
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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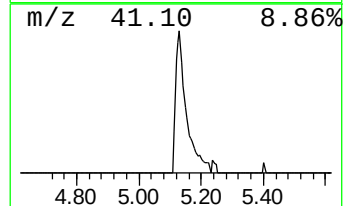
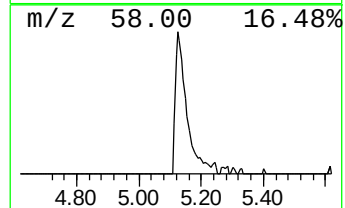
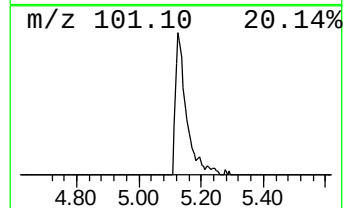
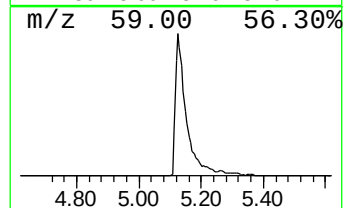
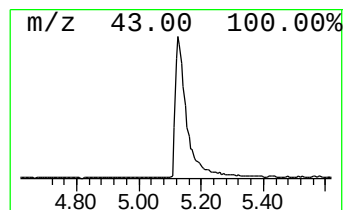
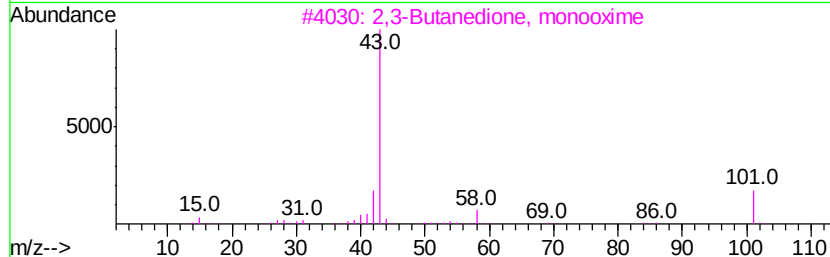
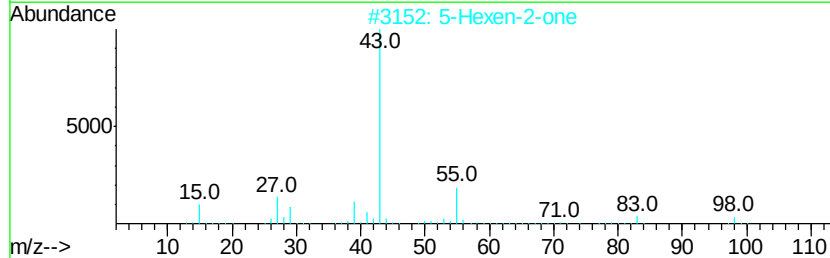
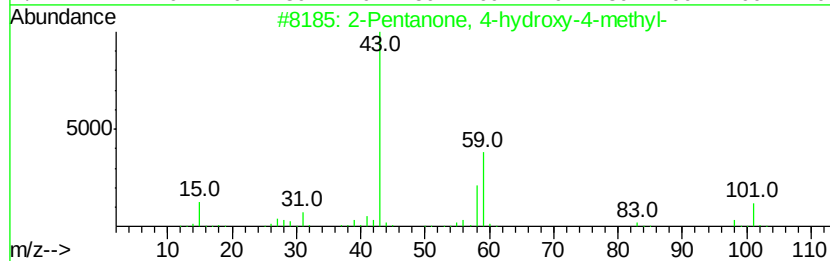
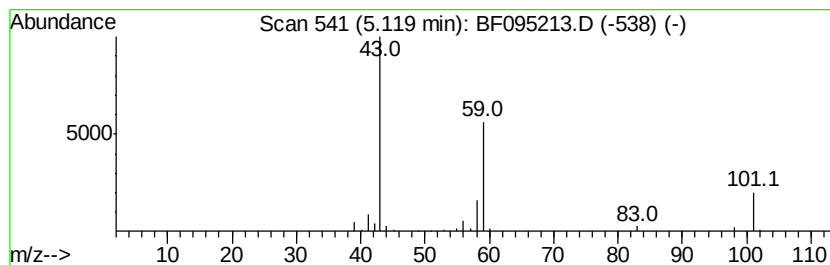
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.12	14.07 ng	334001	1,4-Dichlorobenzene-d4	7.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2		5-Hexen-2-one	98	C6H10O	000109-49-9	9
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9
5		2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	9



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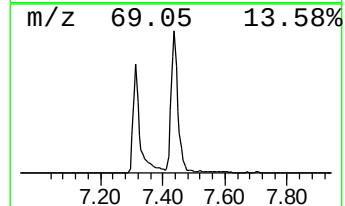
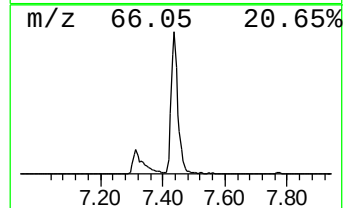
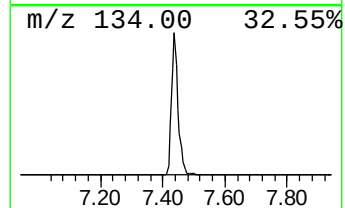
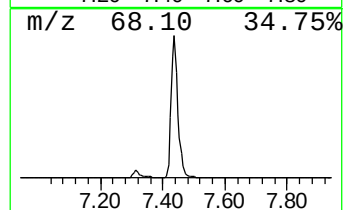
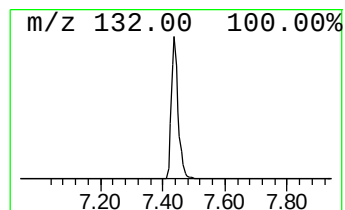
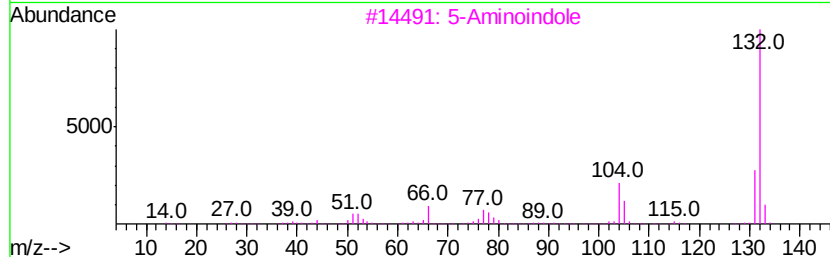
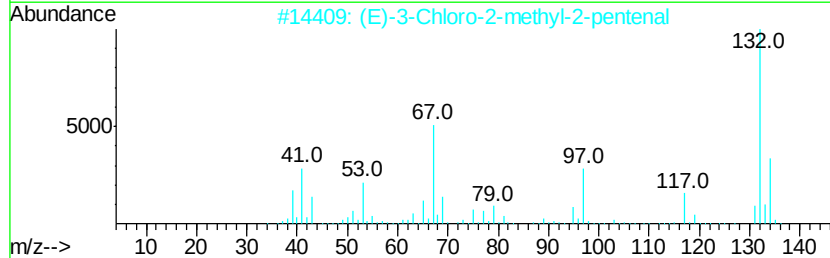
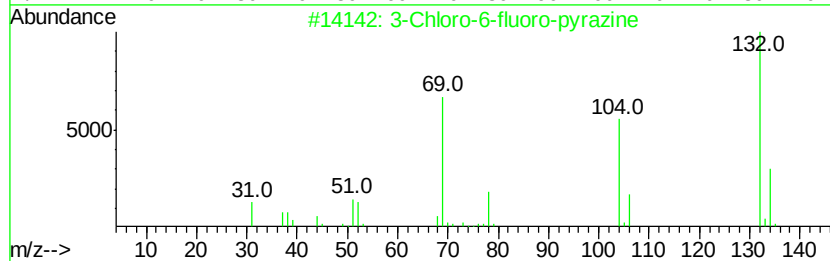
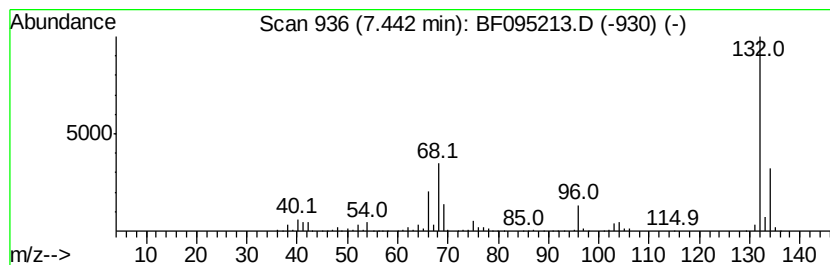
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Peak Number 2 unknown7.44 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.44	99.77 ng	2368480	1,4-Dichlorobenzene-d4	7.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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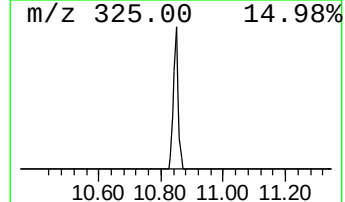
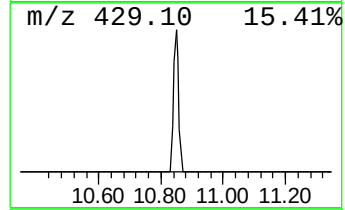
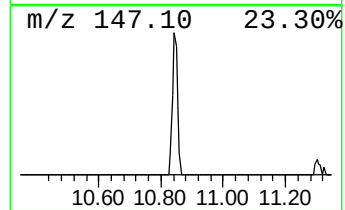
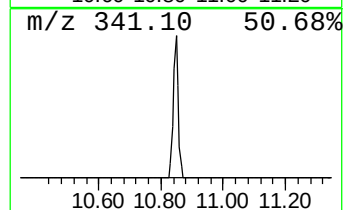
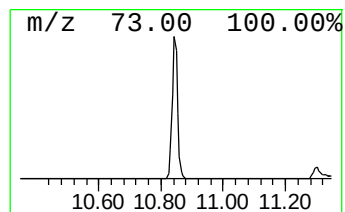
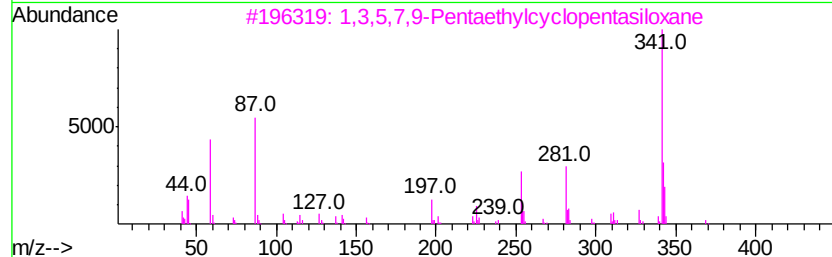
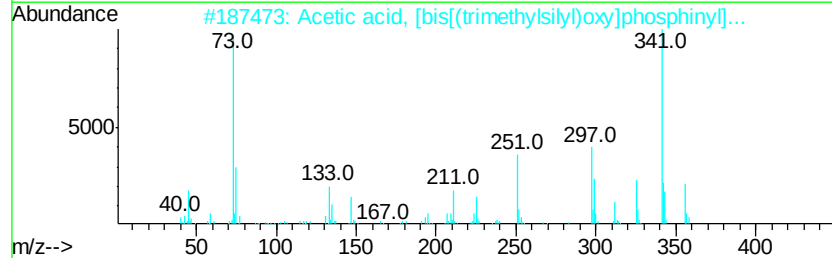
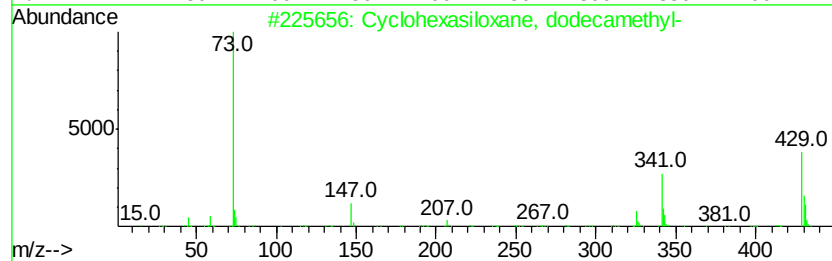
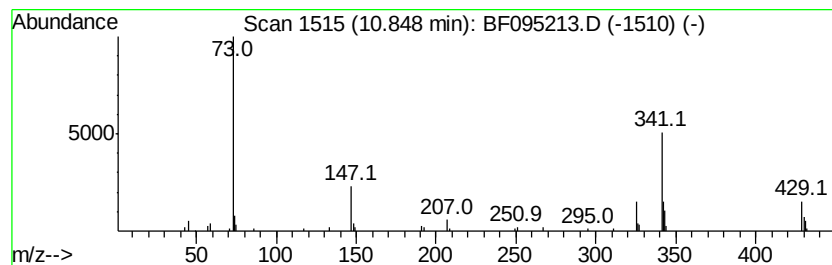
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Peak Number 4 Cyclohexasiloxane, dodecane... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.85	3.26 ng	100122	Naphthalene-d8	9.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexasiloxane, dodecamethyl-	444	C12H36O6Si6	000540-97-6	91
2		Acetic acid, [bis[(trimethylsilyl)oxy]phosphiny]...	356	C11H29O5PSi3	053044-27-2	36
3		1,3,5,7,9-Pentaethylcyclopentasiloxane	370	C10H30O5Si5	017995-44-7	35
4		Morphinan, 7,8-didehydro-4,5-epo...	429	C23H35N03Si2	055449-66-6	18
5		Silane, trimethyl-[[[(17.alpha.)-...	356	C23H36O6Si6	056771-62-1	17



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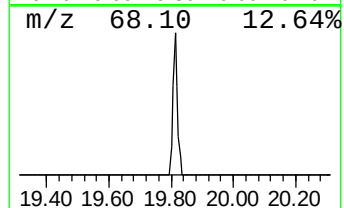
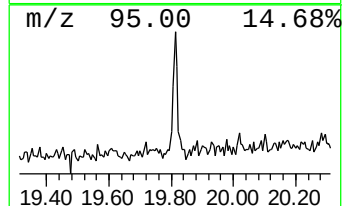
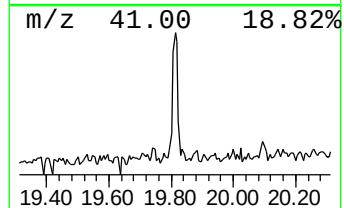
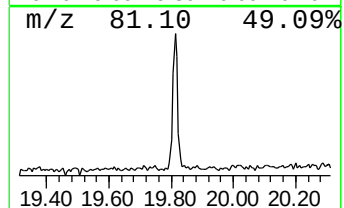
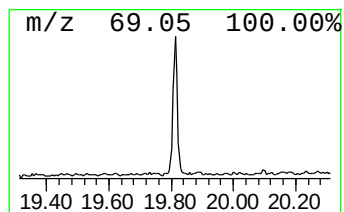
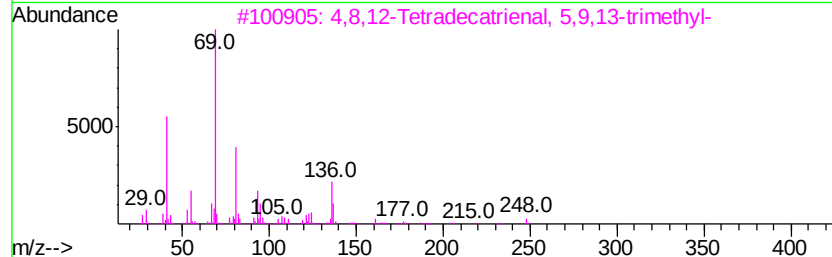
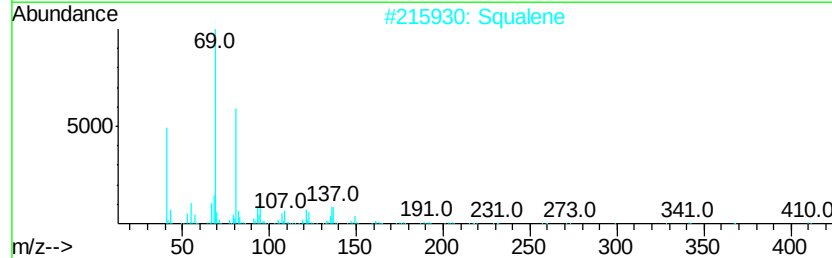
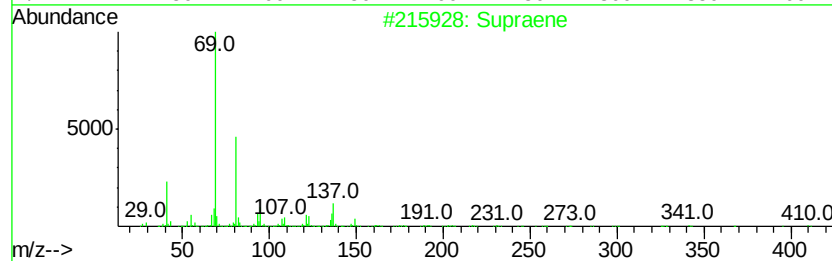
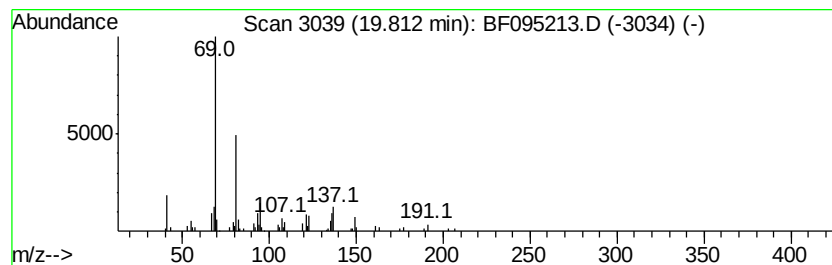
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Peak Number 5 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.81	4.97 ng	89214	Perylene-d12	20.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	91
2		Squalene	410	C30H50	000111-02-4	90
3		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
4		2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64
5		trans-Farnesol	222	C15H26O	000106-28-5	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.12	14.1	ng	334001	1	7.77	474791	20.0
unknown7.44	7.44	99.8	ng	2368480	1	7.77	474791	20.0
Cyclohexasiloxane...	10.85	3.3	ng	100122	2	9.79	614113	20.0
Supraene	19.81	5.0	ng	89214	6	20.37	359118	20.0