

Data Path : U:\HPCHEM1\BNA F\DATA\BF082117\
 Data File : BF097903.D
 Acq On : 21 Aug 2017 13:40
 Operator : SJ/JU
 Sample : I4873-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TEC-BE3-1-3-COMP

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	3.134	175	178	193	rBV	65390	123912	1.76%	0.307%
2	4.951	483	487	496	rVB	260509	355074	5.05%	0.878%
3	5.363	551	557	560	rBV	2836673	2993362	42.55%	7.406%
4	6.387	725	731	735	rBV	2941788	3172568	45.10%	7.849%
5	6.516	748	753	757	rBV	2984890	3009314	42.78%	7.445%
6	6.745	789	792	796	rBV	1007595	854873	12.15%	2.115%
7	6.904	815	819	822	rBV	2574948	2260953	32.14%	5.594%
8	7.310	883	888	891	rBV	1953987	1938030	27.55%	4.795%
9	8.028	1006	1010	1014	rBV	1208628	1104472	15.70%	2.733%
10	9.110	1188	1194	1197	rBV	3364852	3193785	45.40%	7.902%
11	9.498	1256	1260	1264	rBV	464337	359799	5.11%	0.890%
12	9.781	1302	1308	1312	rVB	1313946	1106026	15.72%	2.736%
13	10.569	1437	1442	1445	rBV	1704656	1608766	22.87%	3.980%
14	10.692	1460	1463	1472	rBV	76815	91213	1.30%	0.226%
15	11.263	1556	1560	1563	rBV	1101696	946921	13.46%	2.343%
16	11.833	1653	1657	1660	rVB	1542185	1261588	17.93%	3.121%
17	12.469	1761	1765	1768	rVB	83730	72989	1.04%	0.181%
18	12.692	1797	1803	1807	rBV	67492	75972	1.08%	0.188%
19	12.845	1825	1829	1833	rBV	2159676	2052310	29.18%	5.078%
20	13.321	1907	1910	1914	rBV	240045	228817	3.25%	0.566%
21	13.745	1977	1982	1987	rBV2	182264	245299	3.49%	0.607%
22	13.898	2002	2008	2011	rBV2	5463012	7034393	100.00%	17.404%
23	14.286	2071	2074	2076	rBV	86501	85501	1.22%	0.212%
24	14.468	2102	2105	2108	rVB	83444	76046	1.08%	0.188%
25	14.504	2108	2111	2114	rBV	106208	112949	1.61%	0.279%
26	14.745	2149	2152	2155	rVB	88945	96974	1.38%	0.240%
27	14.904	2176	2179	2182	rBV2	51553	72911	1.04%	0.180%
28	15.310	2243	2248	2254	rBV	586737	739314	10.51%	1.829%
29	17.445	2586	2611	2630	rVB4	809027	5144663	73.14%	12.728%

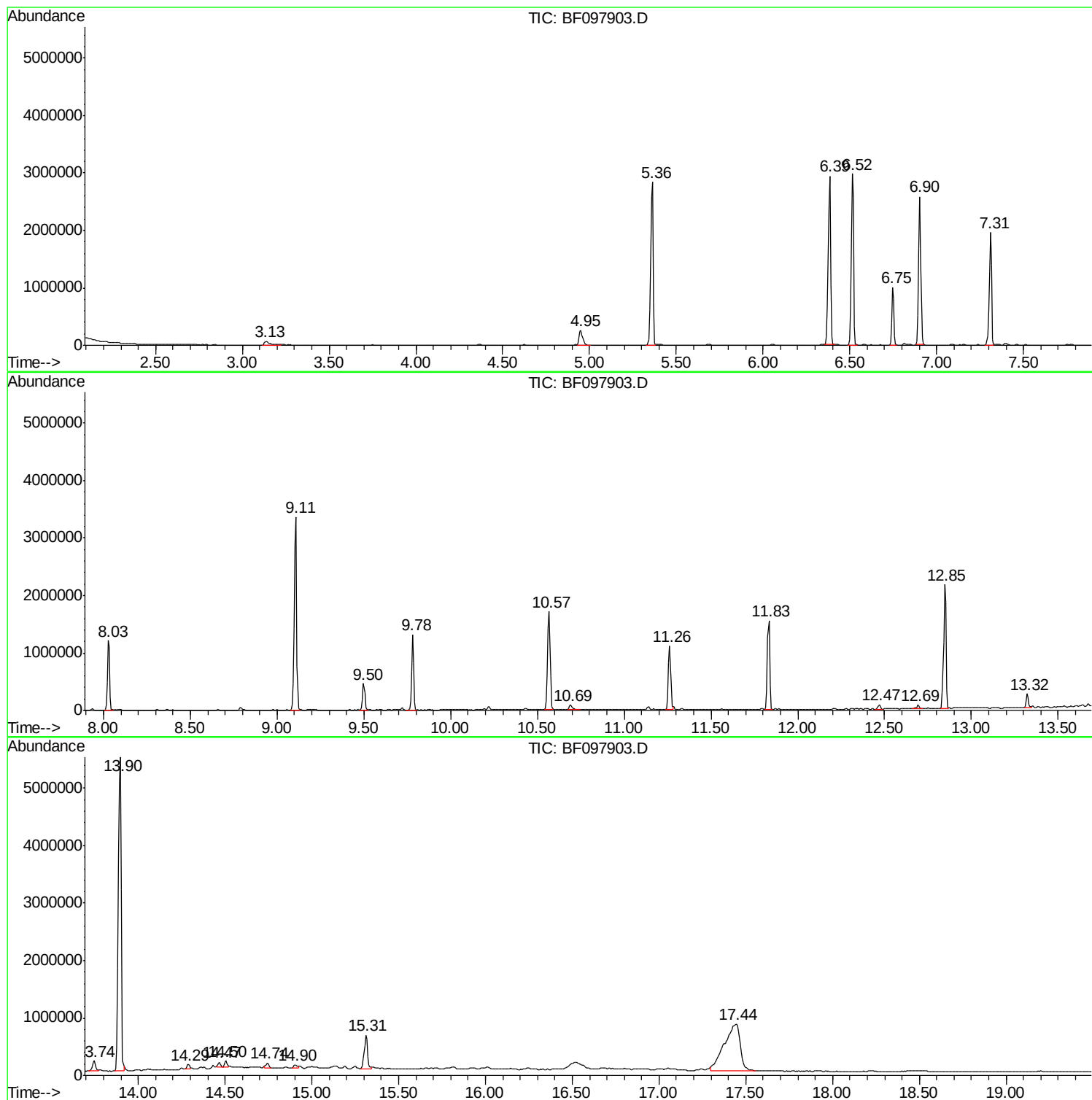
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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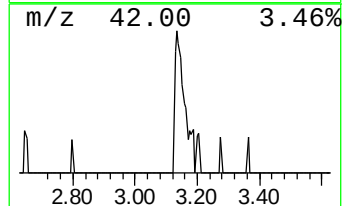
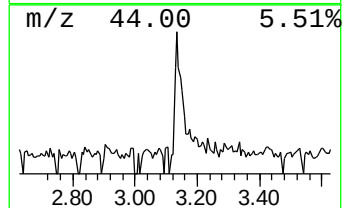
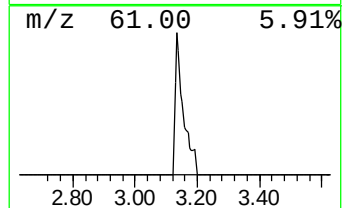
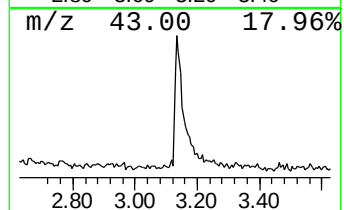
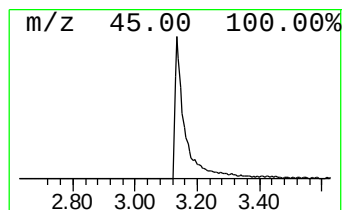
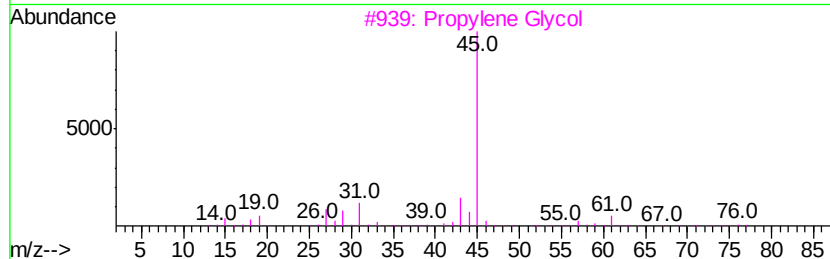
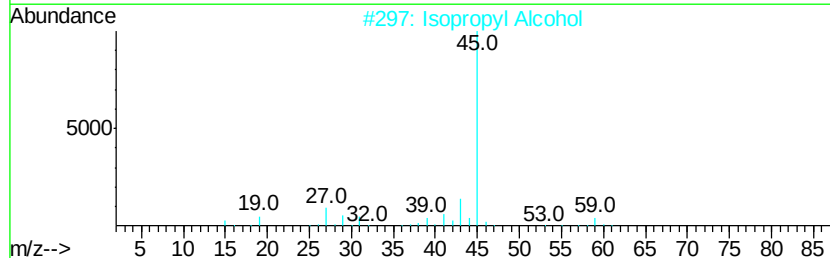
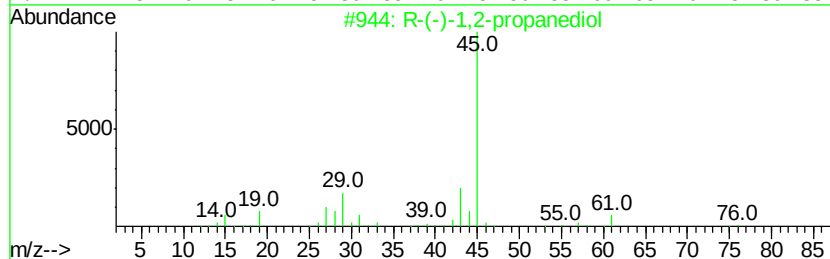
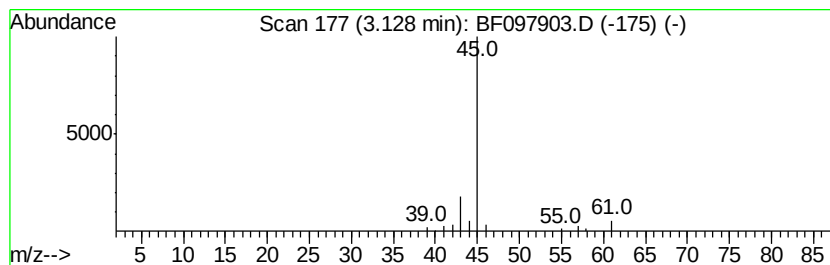
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.13 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	2.90 ng	123912	1,4-Dichlorobenzene-d4	6.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
2		Isopropyl Alcohol	60	C3H8O	000067-63-0	9
3		Propylene Glycol	76	C3H8O2	000057-55-6	9
4		L-Lactic acid	90	C3H6O3	000079-33-4	9
5		(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9



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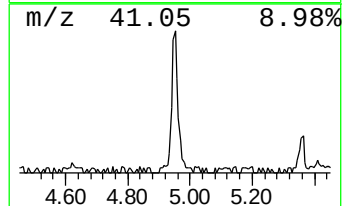
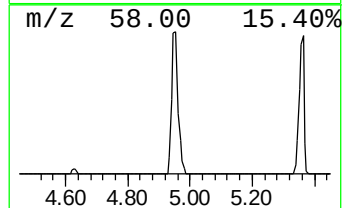
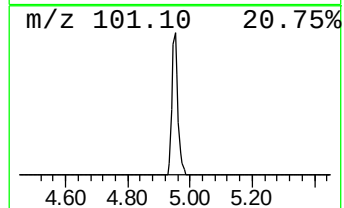
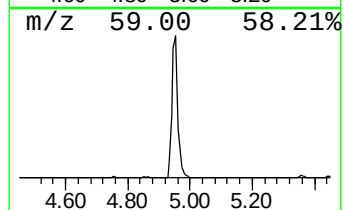
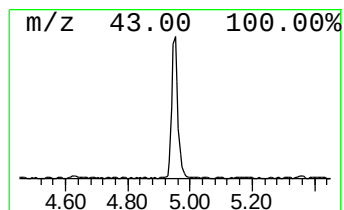
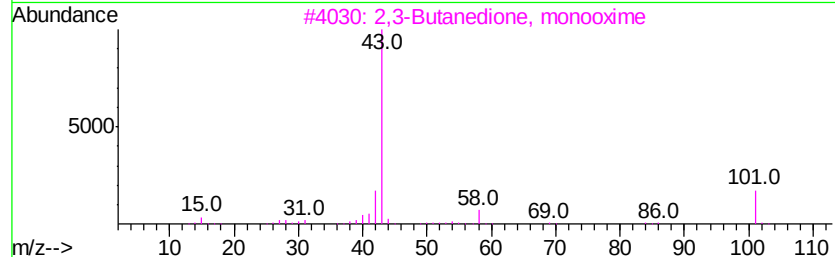
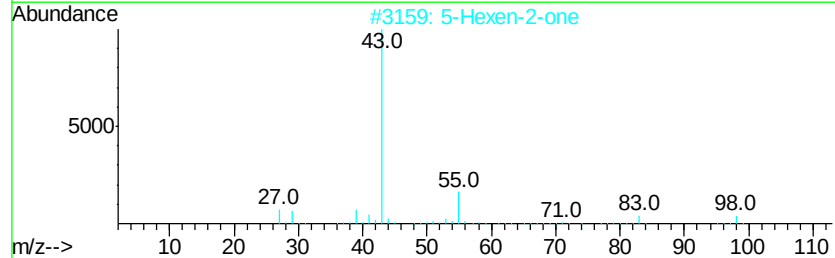
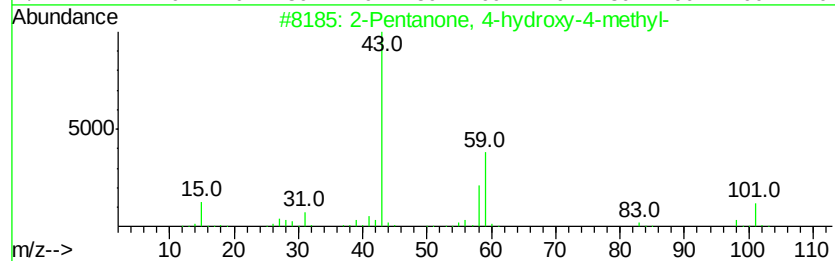
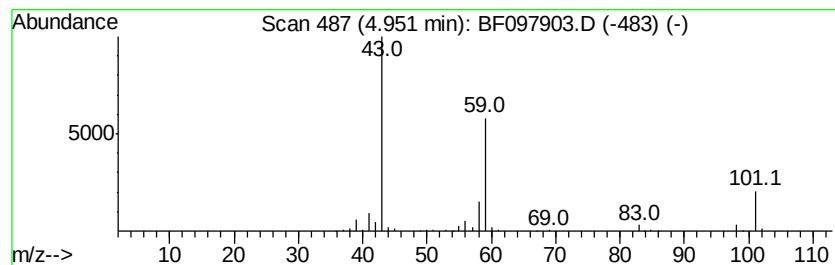
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.95	8.31 ng	355074	1,4-Dichlorobenzene-d4	6.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		5-Hexen-2-one	98	C6H10O	000109-49-9	9
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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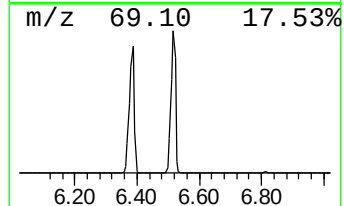
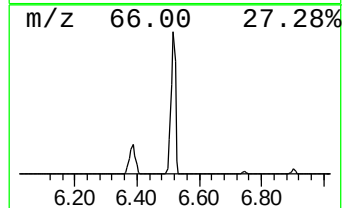
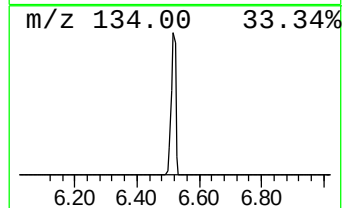
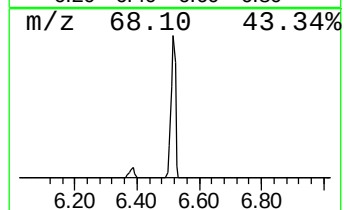
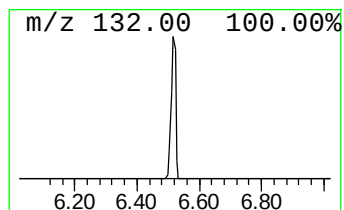
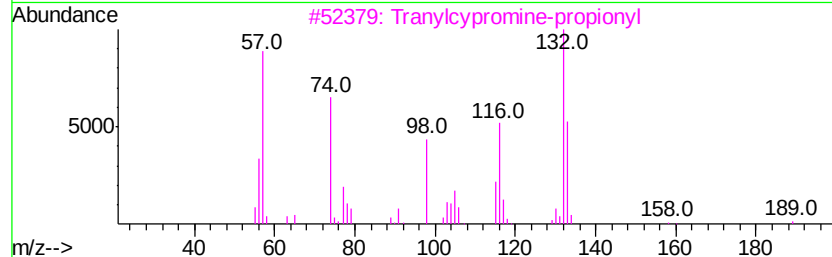
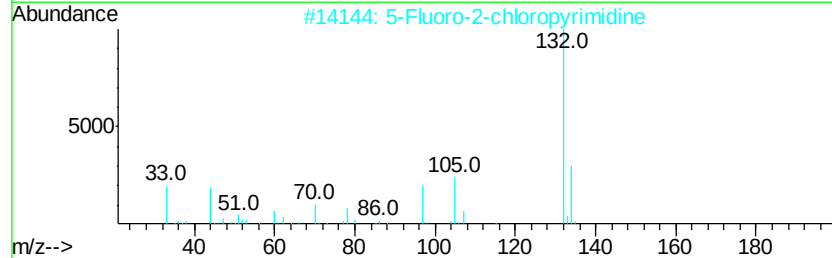
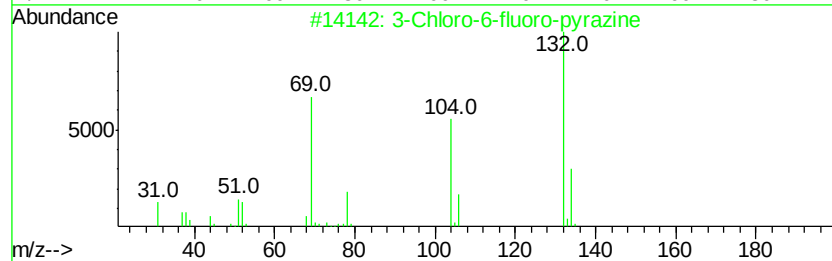
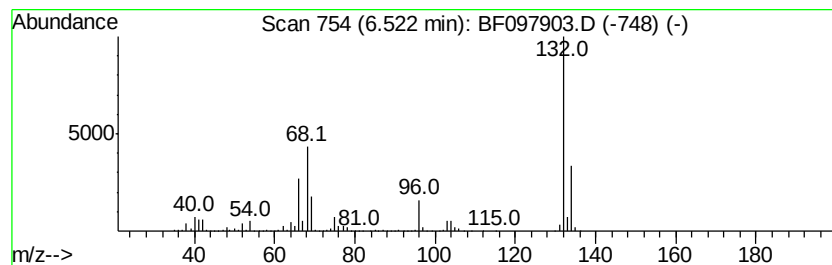
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Peak Number 3 unknown6.52 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	70.40 ng	3009310	1,4-Dichlorobenzene-d4	6.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		Tranvlcypropamine-propionyl	189	C12H15NO	1000123-86-3	10
4		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5		Xenon	132	Xe	007440-63-3	9



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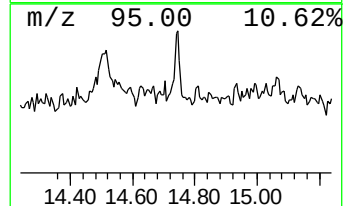
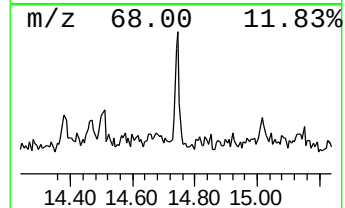
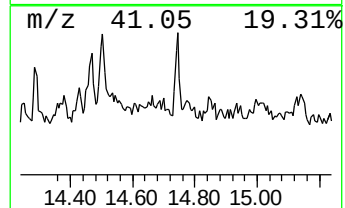
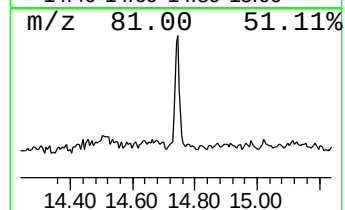
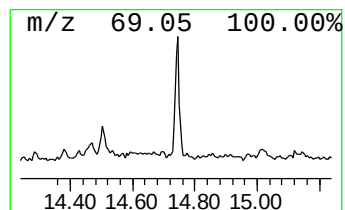
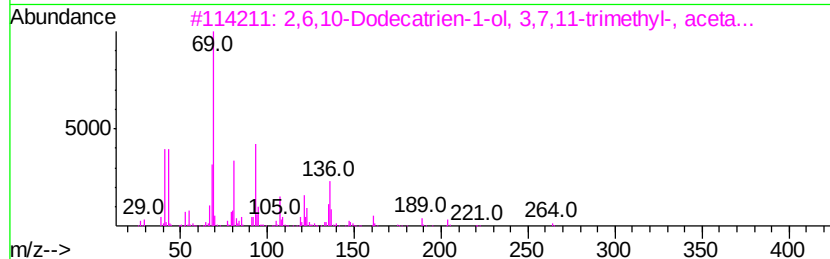
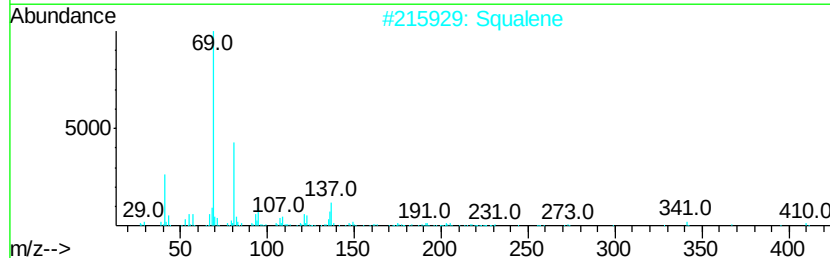
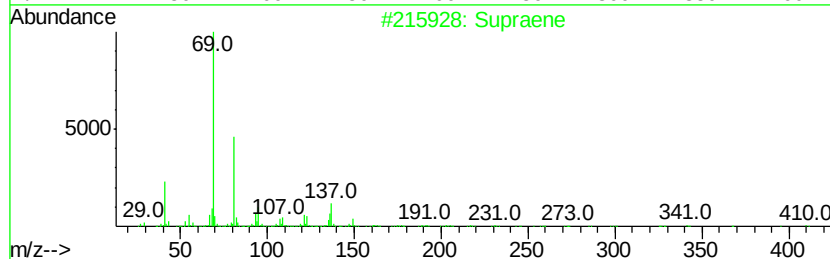
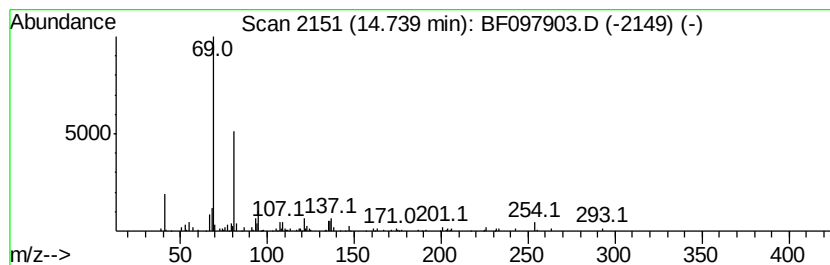
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Peak Number 5 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.74	2.62 ng	96974	Perylene-d12	15.31

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene		410	C30H50	007683-64-9	87
2	Squalene		410	C30H50	000111-02-4	78
3	2,6,10-Dodecatrien-1-ol, 3,7,11-...		264	C17H28O2	004128-17-0	78
4	trans-Farnesol		222	C15H26O	000106-28-5	74
5	1,6-Octadiene, 2,7-dimethyl-		138	C10H18	040195-09-3	53



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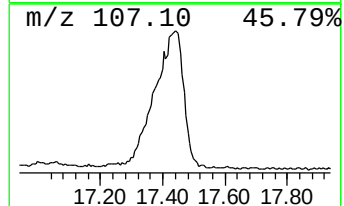
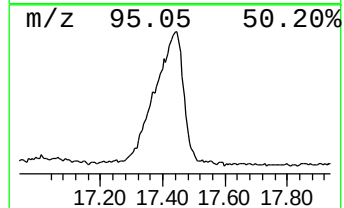
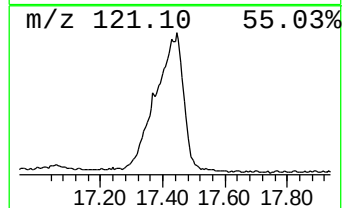
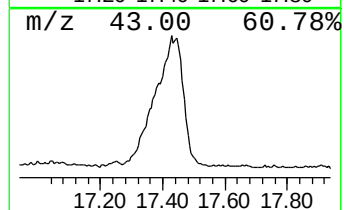
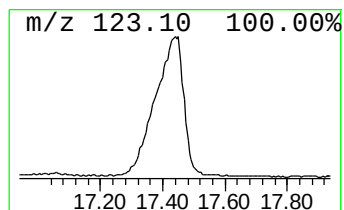
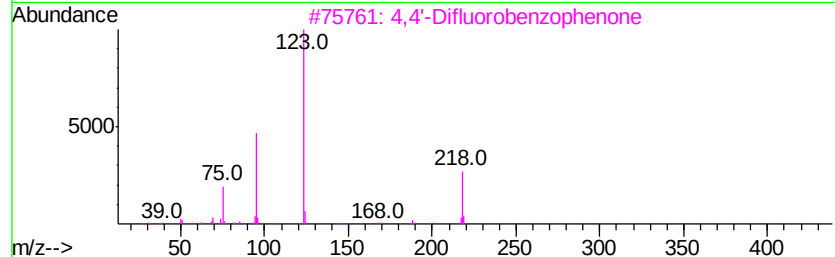
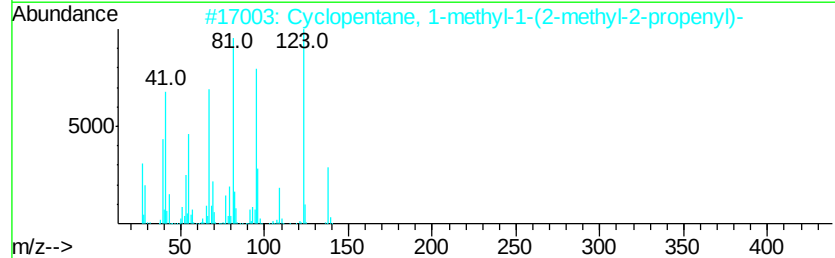
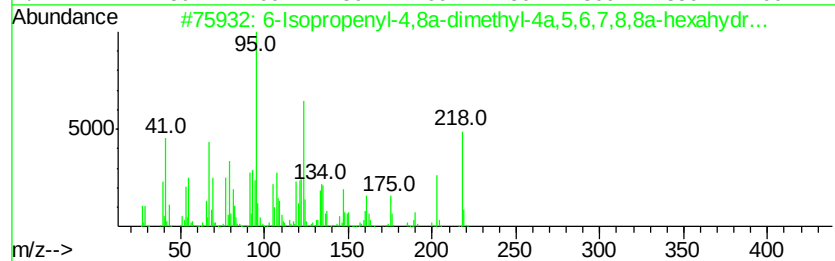
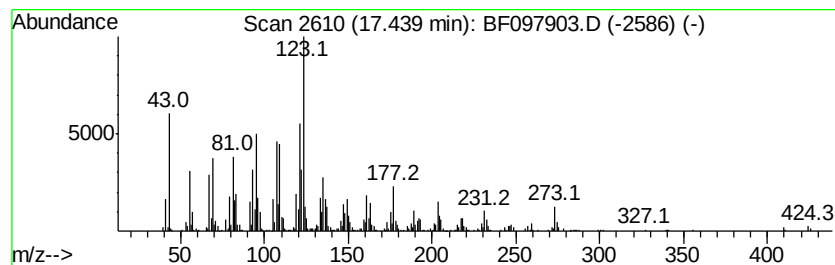
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Peak Number 6 unknown17.44 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.44	139.17 ng	5144660	Perylene-d12	15.31

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	6-Isopropenyl-4,8a-dimethyl-4a,5...	218	C15H22O	086917-79-5	41
2		Cyclopentane, 1-methyl-1-(2-meth...	138	C10H18	074764-47-9	35
3		4,4'-Difluorobenzophenone	218	C13H8F2O	000345-92-6	30
4		2-Fluorobenzoic acid, 2,7-dimeth...	274	C17H19F02	1000299-16-7	27
5		4-Fluorobenzoic acid, 2-ethylcyc...	250	C15H19F02	1000279-06-0	27



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown3.13	3.13	2.9	ng	123912	1	6.75	854873	20.0
2-Pentanone, 4-hy...	4.95	8.3	ng	355074	1	6.75	854873	20.0
unknown6.52	6.52	70.4	ng	3009310	1	6.75	854873	20.0
Supraene	14.74	2.6	ng	96974	6	15.31	739314	20.0
unknown17.44	17.44	139.2	ng	5144660	6	15.31	739314	20.0