

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF083116\
 Data File : BF089951.D
 Acq On : 31 Aug 2016 15:36
 Operator : UM/SJ
 Sample : H4620-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RICHMOND-REC-SELECT-FILL

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-BF083116.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	1.633	3	4	13	rVB	222508	513495	6.12%	1.075%
2	1.758	13	15	61	rVB	2711874	8395907	100.00%	17.579%
3	4.764	275	278	285	rVB	728905	1025981	12.22%	2.148%
4	5.210	314	317	319	rBV	3448728	3515125	41.87%	7.360%
5	6.273	407	410	413	rBV	3080007	3488407	41.55%	7.304%
6	6.399	418	421	424	rBV	3745014	3546212	42.24%	7.425%
7	6.639	439	442	444	rBV	1430355	1479463	17.62%	3.098%
8	6.787	453	455	457	rBV	2468038	2763902	32.92%	5.787%
9	7.199	488	491	494	rBV	2158129	2127408	25.34%	4.454%
10	7.919	552	554	557	rBV	2154357	1850785	22.04%	3.875%
11	8.993	646	648	651	rBV	2874469	3992819	47.56%	8.360%
12	9.393	681	683	685	rBV	1398941	1138027	13.55%	2.383%
13	9.668	704	707	709	rBV	1948760	1949601	23.22%	4.082%
14	10.445	772	775	777	rBV	2099887	1942195	23.13%	4.066%
15	10.582	786	787	792	rVB	99016	148235	1.77%	0.310%
16	11.131	833	835	839	rVV	1601153	1667590	19.86%	3.491%
17	12.331	938	940	943	rVB	151737	136295	1.62%	0.285%
18	12.559	956	960	961	rBV	129357	172801	2.06%	0.362%
19	12.719	971	974	976	rBV	2833774	2919576	34.77%	6.113%
20	13.634	1051	1054	1057	rBV2	123255	194312	2.31%	0.407%
21	13.748	1061	1064	1070	rBV	1749032	1831158	21.81%	3.834%
22	14.262	1106	1109	1112	rBV3	65711	129396	1.54%	0.271%
23	14.731	1148	1150	1155	rVB	66385	117716	1.40%	0.246%
24	14.834	1157	1159	1161	rBV2	55985	88610	1.06%	0.186%
25	15.097	1179	1182	1185	rBV	1477532	1669334	19.88%	3.495%
26	18.537	1478	1483	1493	rVB	320168	957359	11.40%	2.004%

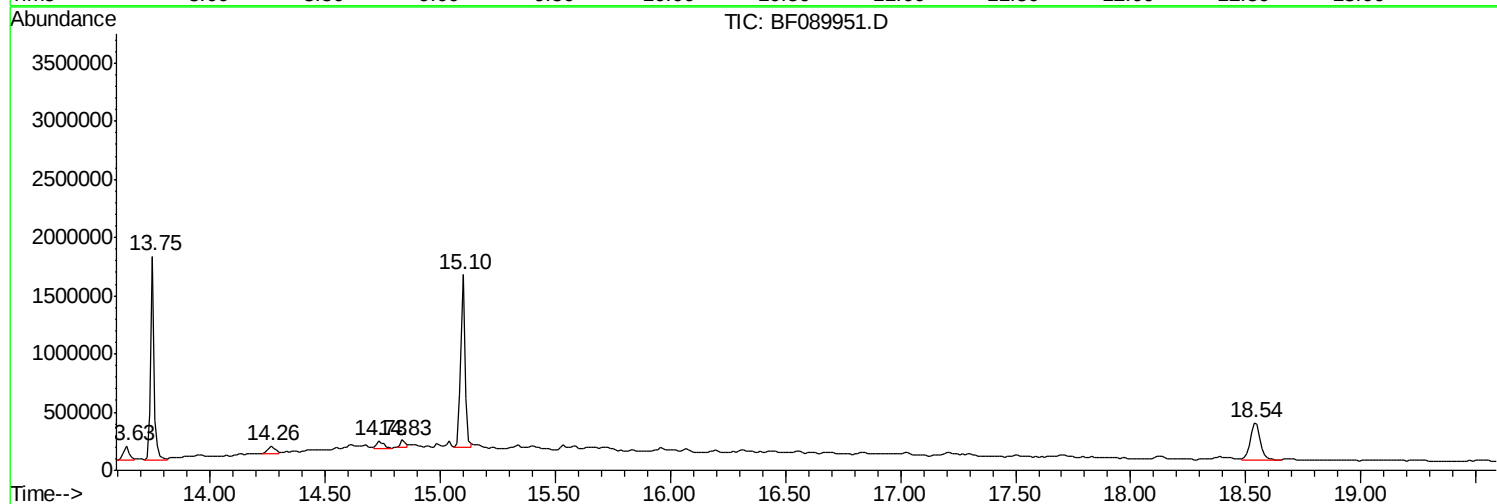
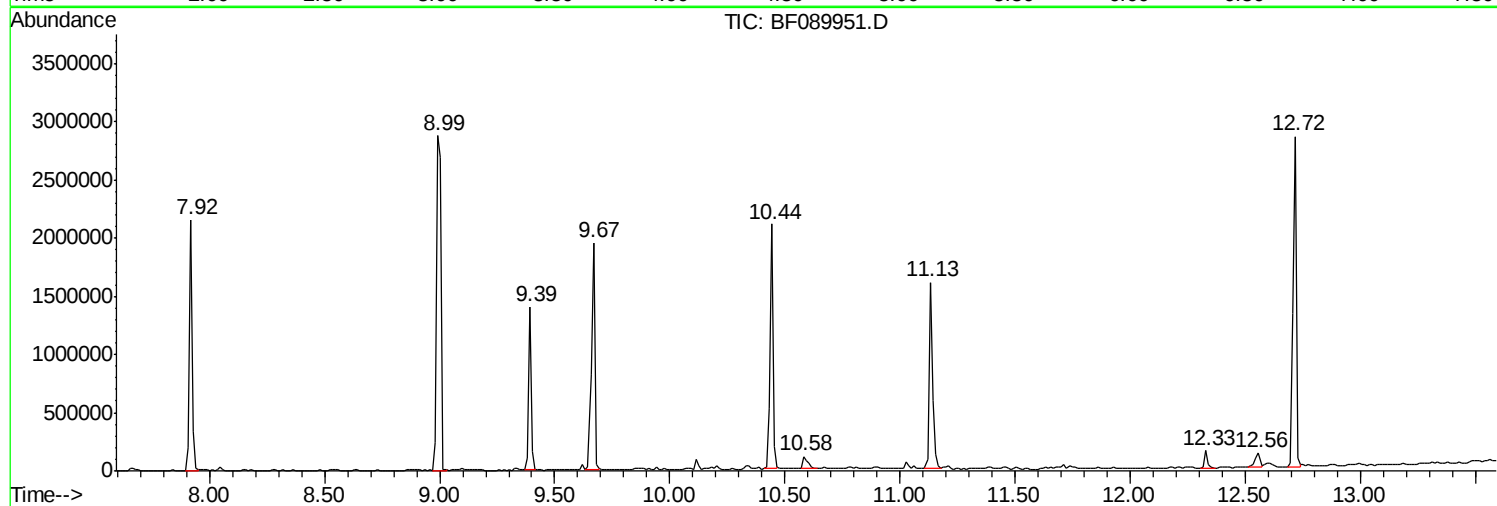
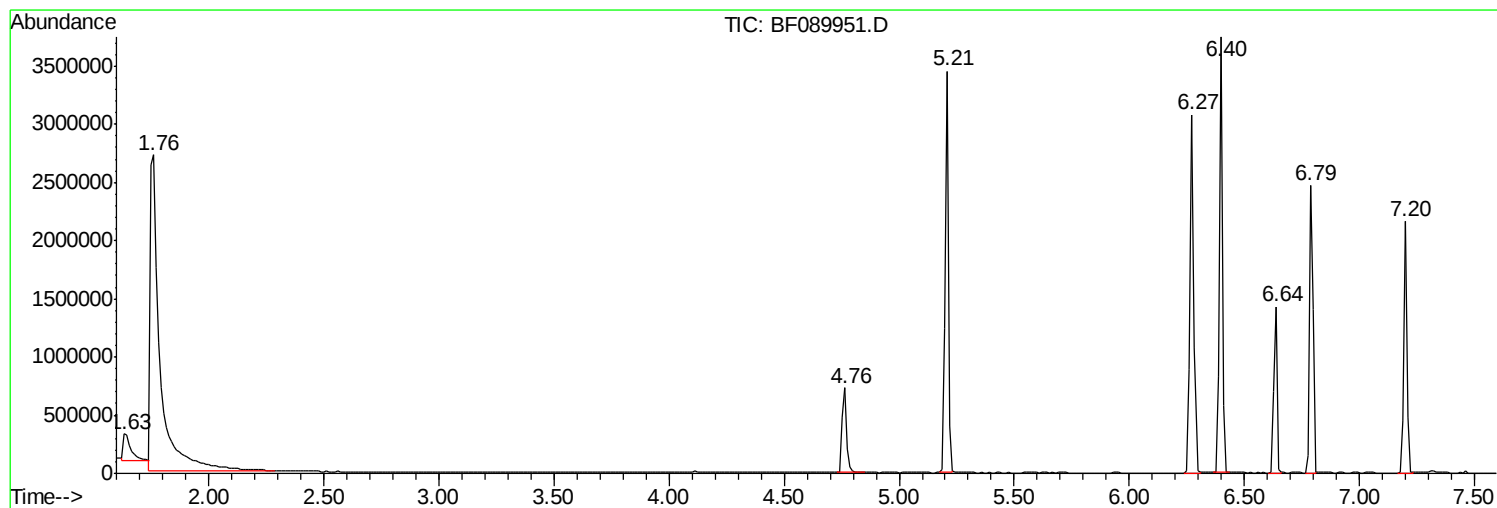
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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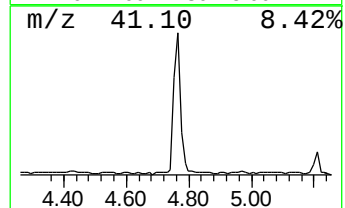
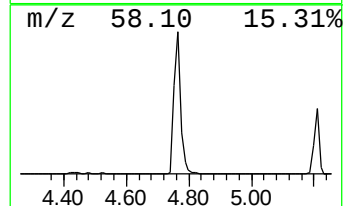
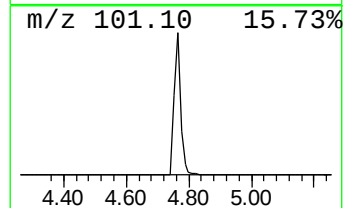
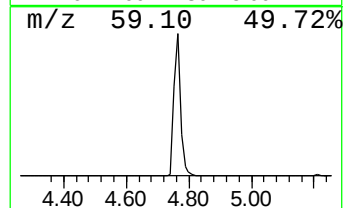
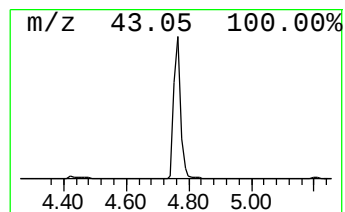
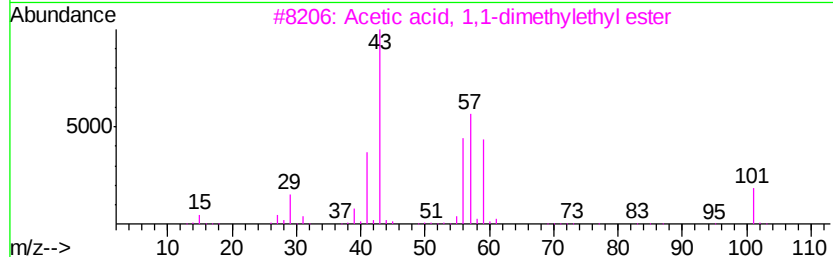
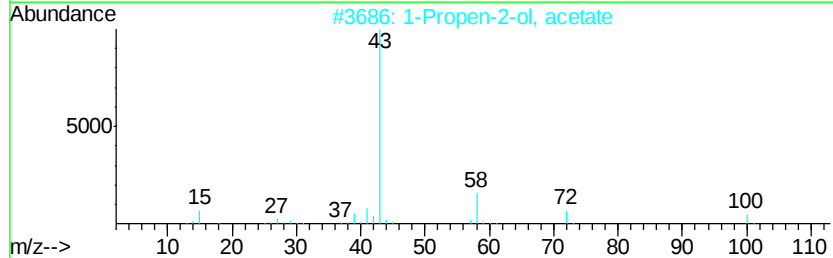
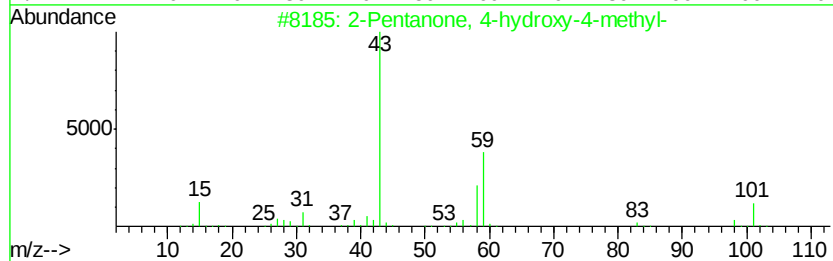
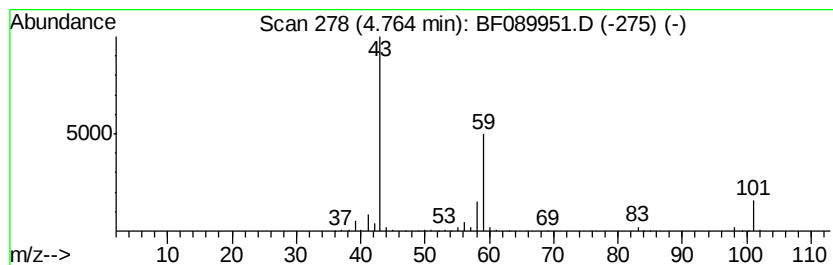
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.76	13.87 ng	1025980	1,4-Dichlorobenzene-d4	6.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
4		Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	7
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	7



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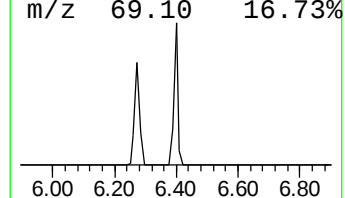
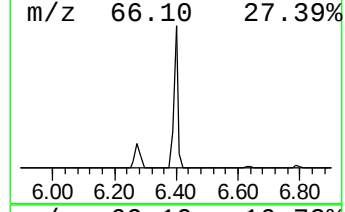
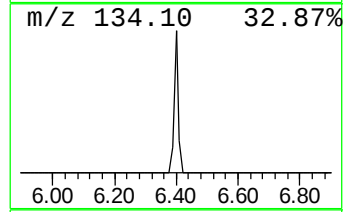
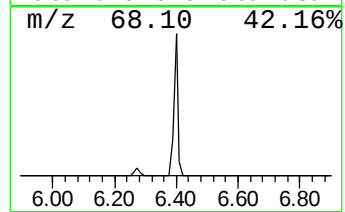
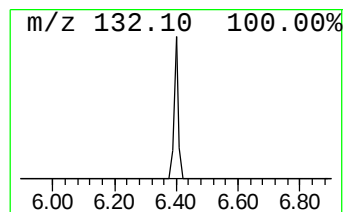
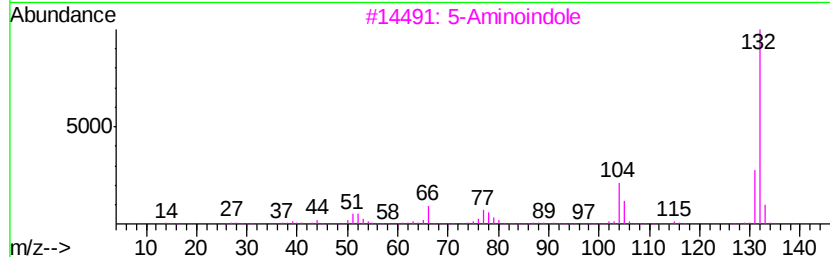
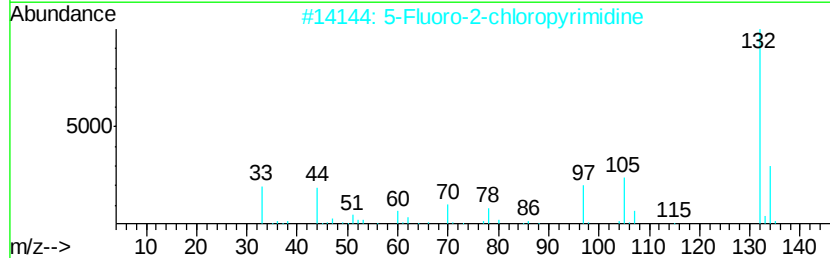
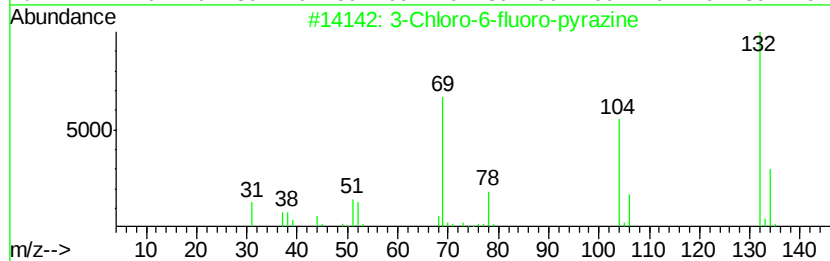
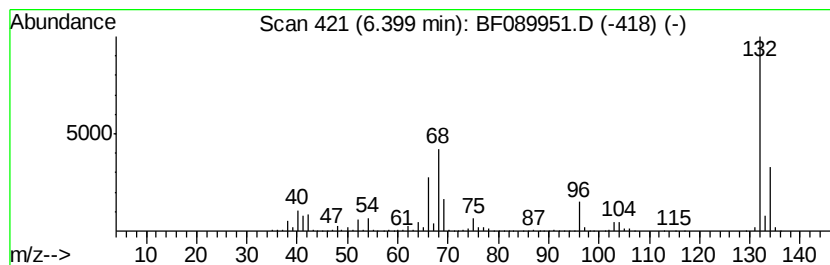
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Peak Number 4 unknown6.40 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.40	47.94 ng	3546210	1,4-Dichlorobenzene-d4	6.64

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	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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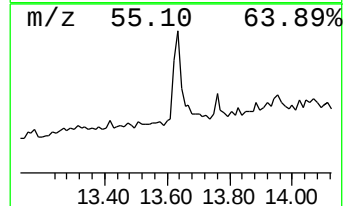
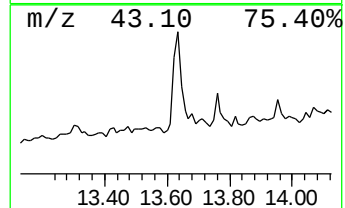
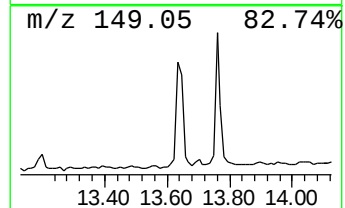
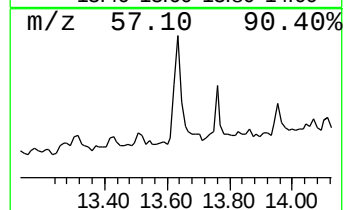
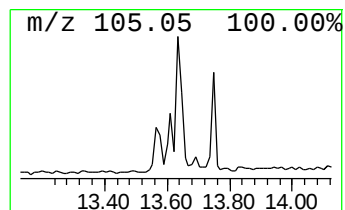
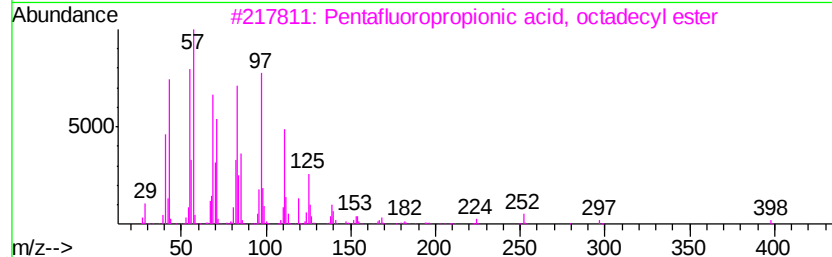
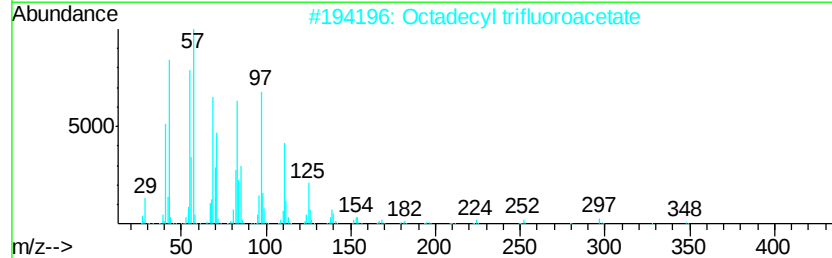
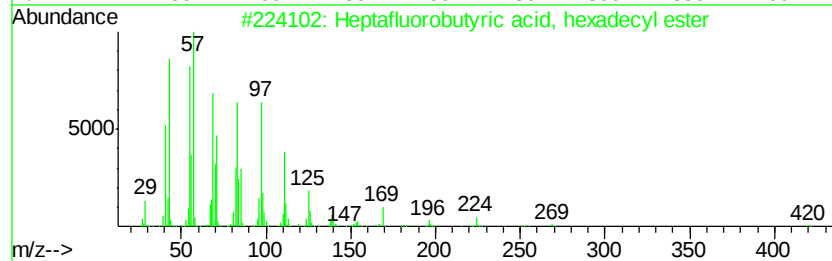
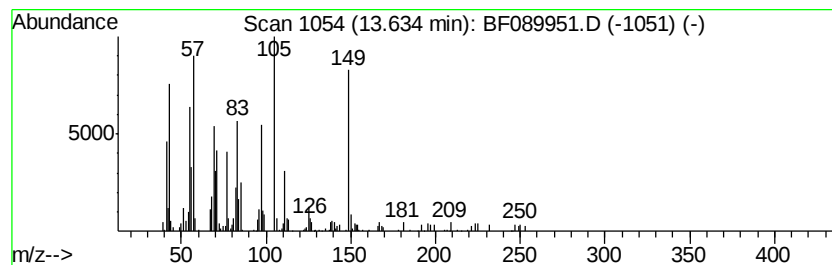
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Peak Number 6 Heptafluorobutyric acid, he... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.63	2.12 ng	194312	Chrysene-d12	13.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	50
2		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	50
3		Pentafluoropropionic acid, octadec...	416	C21H37F5O2	959261-25-7	50
4		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	50
5		1-Heptacosanol	396	C27H56O	002004-39-9	50



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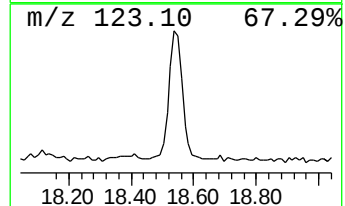
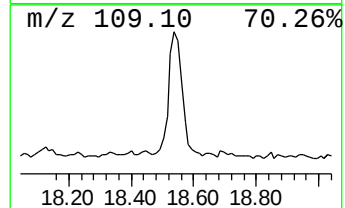
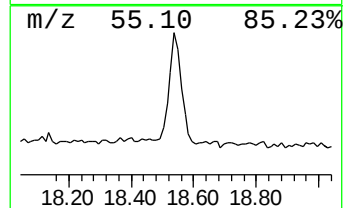
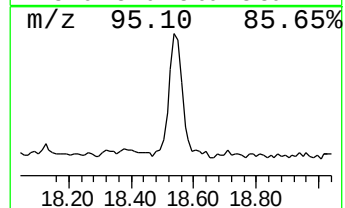
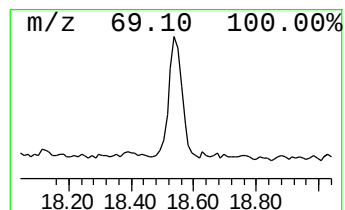
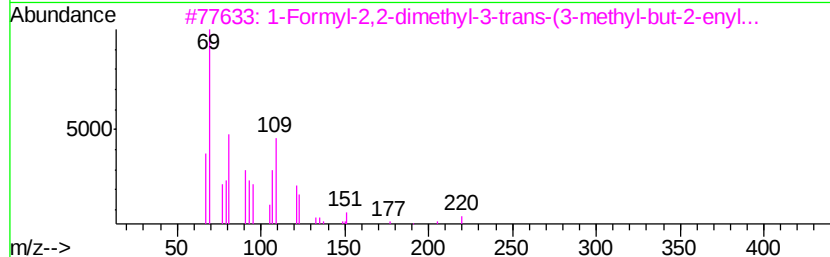
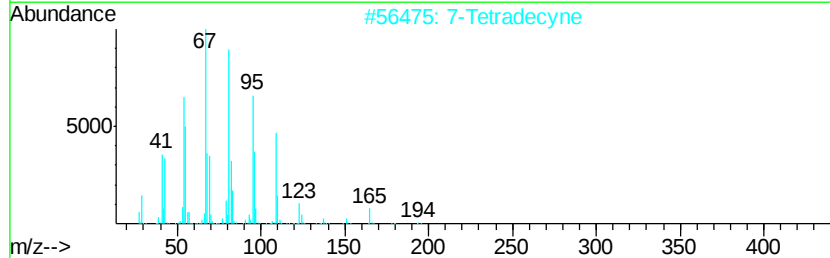
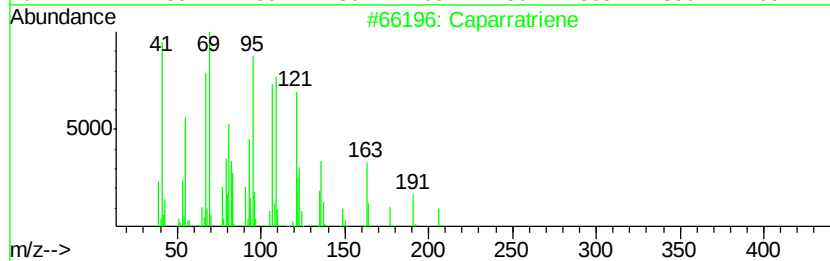
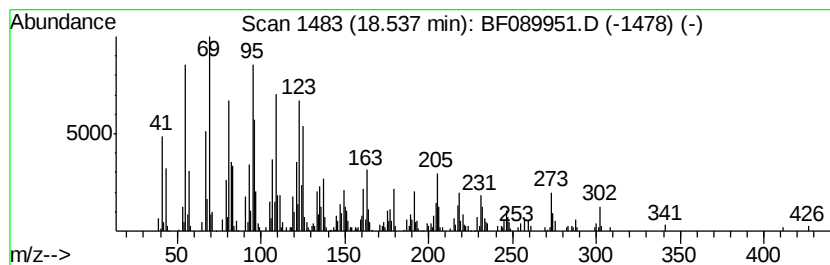
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Peak Number 7 Caparratriene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.54	11.47 ng	957359	Perylene-d12	15.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Caparratriene	206	C15H26	1000374-08-7	53
2		7-Tetradecyne	194	C14H26	035216-11-6	38
3		1-Formyl-2,2-dimethyl-3-trans-(3...	220	C15H24O	1000144-09-7	30
4		Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	000473-19-8	25
5		6-Isopropenyl-4,8a-dimethyl-4a,5...	218	C15H22O	086917-79-5	25



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.76	13.9	ng	1025980	1	6.64	1479460	20.0
unknown6.40	6.40	47.9	ng	3546210	1	6.64	1479460	20.0
Heptafluorobutyri...	13.63	2.1	ng	194312	5	13.75	1831160	20.0
Caparratriene	18.54	11.5	ng	957359	6	15.10	1669330	20.0