

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF070318\
 Data File : BF107113.D
 Acq On : 4 Jul 2018 6:12
 Operator : JU/SJ
 Sample : J3804-04
 Misc :
 ALS Vial : 42 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-02

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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	5.184	481	484	491	rBV	45928	52603	3.18%	0.518%
2	5.601	551	555	573	rVB	599971	605204	36.59%	5.965%
3	6.601	722	725	740	rVB	369759	390779	23.62%	3.852%
4	6.736	743	748	751	rBV	1167835	1092083	66.02%	10.764%
5	6.954	781	785	788	rBV	384517	304053	18.38%	2.997%
6	7.113	808	812	815	rBV	1199270	1073525	64.90%	10.581%
7	7.525	877	882	885	rBV	889141	833538	50.39%	8.216%
8	8.236	1000	1003	1008	rBV	380777	331751	20.06%	3.270%
9	8.472	1040	1043	1046	rVB	55051	41398	2.50%	0.408%
10	9.313	1181	1186	1201	rBV	1450339	1432402	86.60%	14.118%
11	9.701	1249	1252	1258	rBV	62062	60107	3.63%	0.592%
12	9.995	1298	1302	1315	rVB2	360304	354136	21.41%	3.490%
13	10.236	1341	1343	1347	rVB2	20060	19852	1.20%	0.196%
14	10.795	1434	1438	1443	rBV	925248	867668	52.45%	8.552%
15	11.448	1544	1549	1553	rBV	11735	16768	1.01%	0.165%
16	11.489	1553	1556	1563	rVB	417524	378203	22.86%	3.728%
17	13.077	1821	1826	1829	rBV	1703590	1654127	100.00%	16.304%
18	13.948	1971	1974	1980	rVB	42346	45592	2.76%	0.449%
19	14.142	2003	2007	2016	rVB	351898	353761	21.39%	3.487%
20	15.683	2265	2269	2275	rVB	174443	238271	14.40%	2.348%

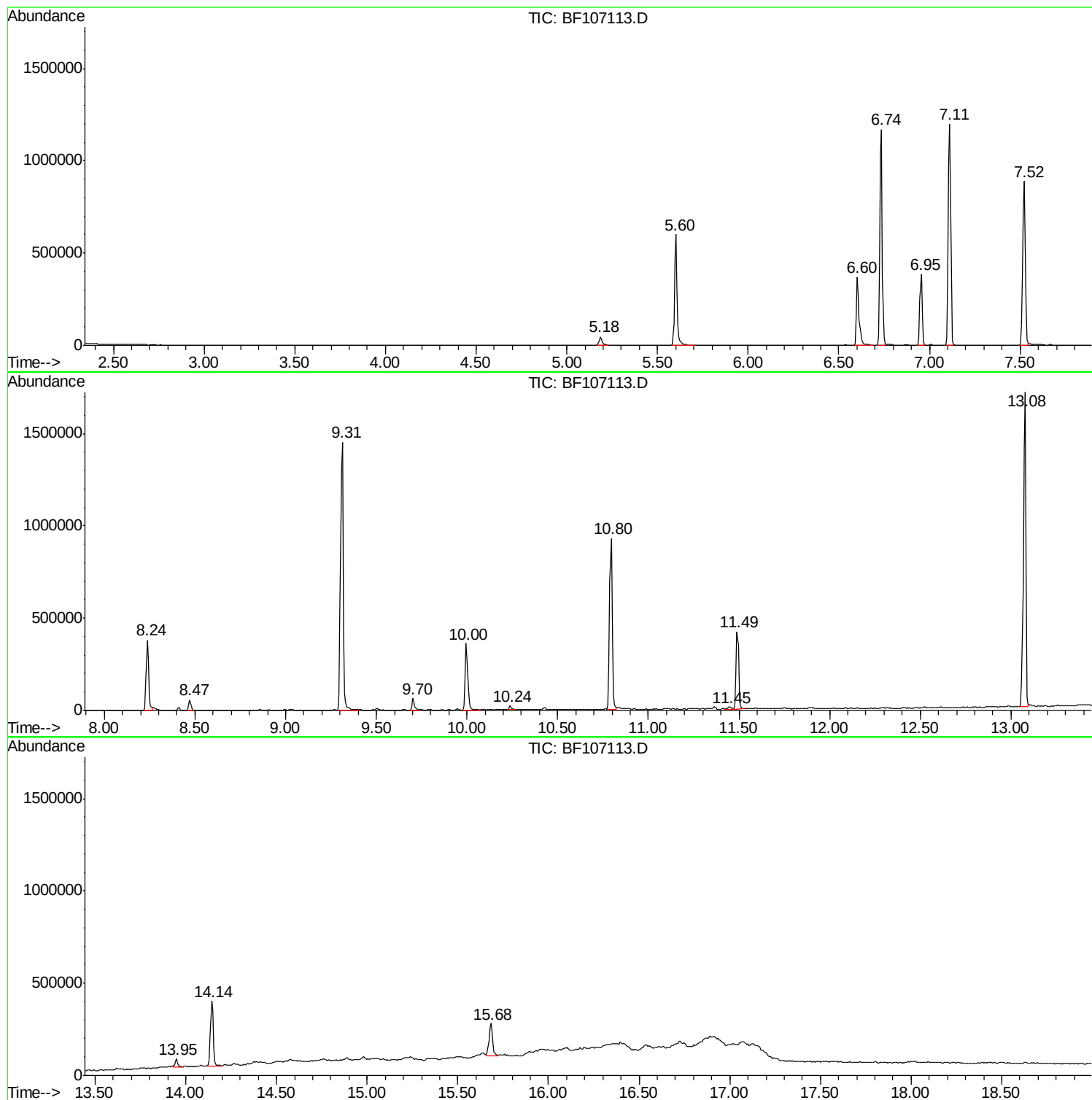
Sum of corrected areas: 10145821

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.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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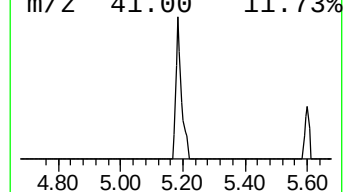
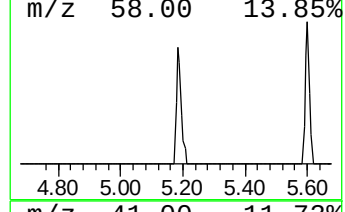
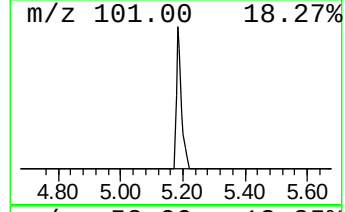
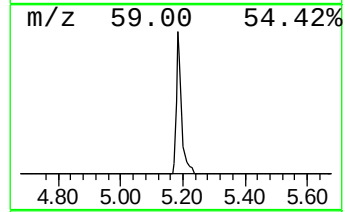
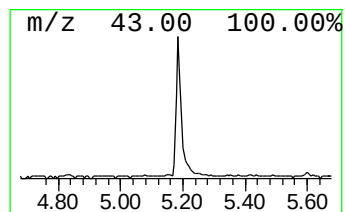
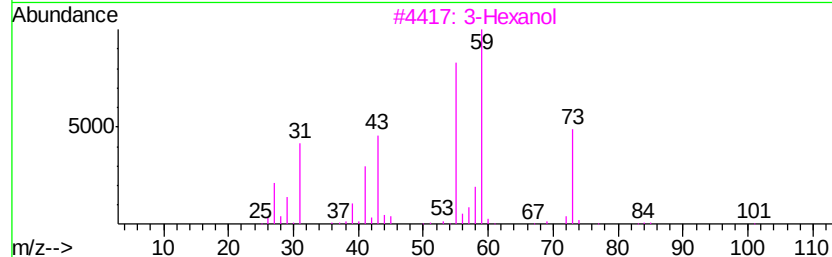
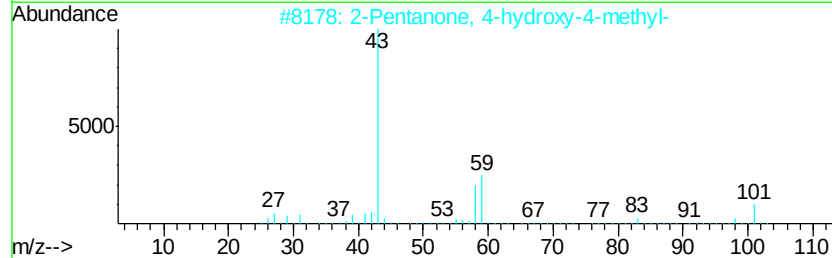
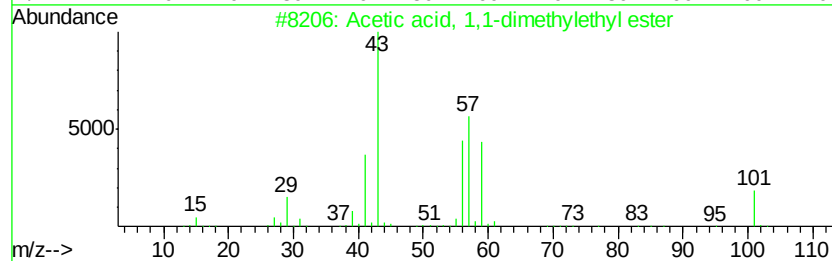
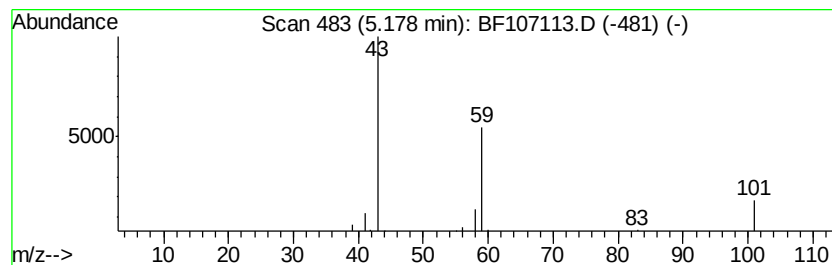
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Acetic acid, 1,1-dimethylet... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	3.46 ng	52603	1,4-Dichlorobenzene-d4	6.95

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	50
2			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
3			3-Hexanol	102	C6H14O	000623-37-0	28
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23



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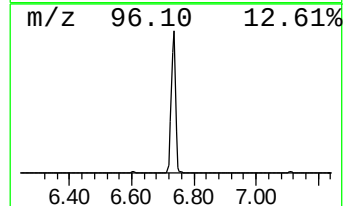
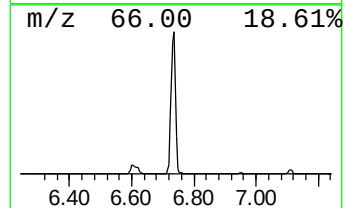
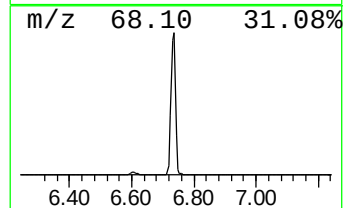
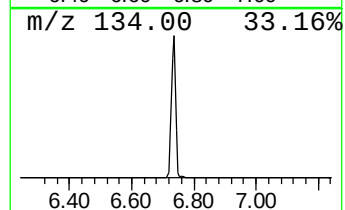
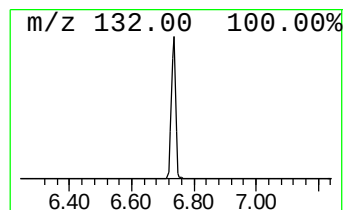
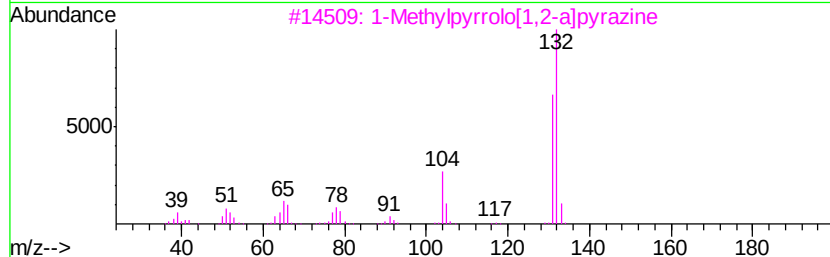
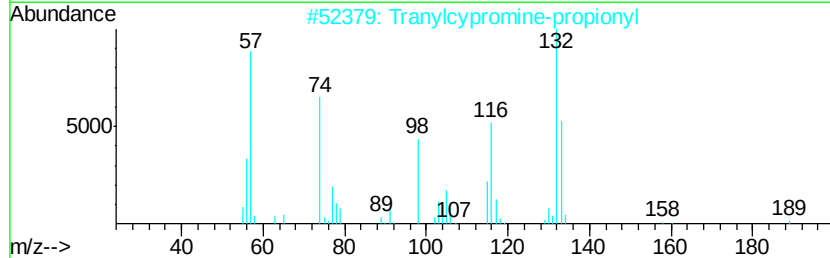
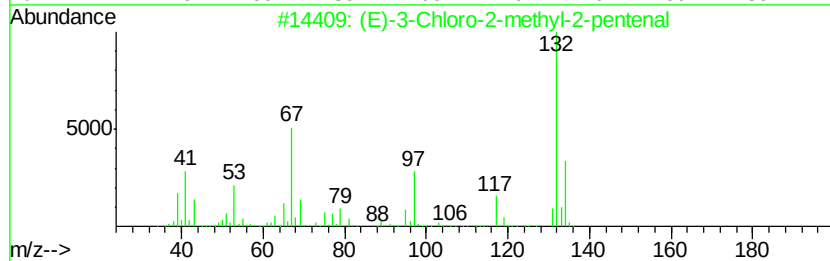
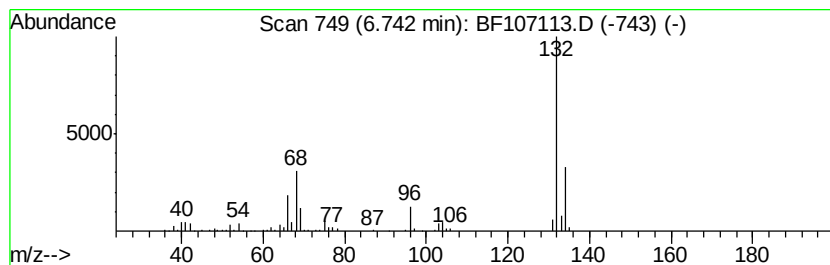
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Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	71.84 ng	1092080	1,4-Dichlorobenzene-d4	6.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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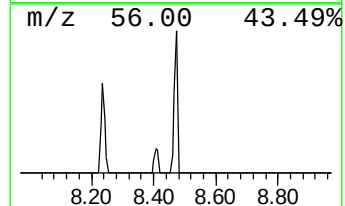
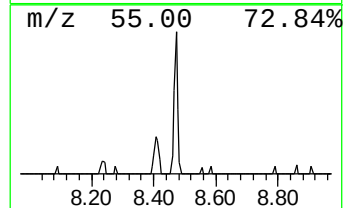
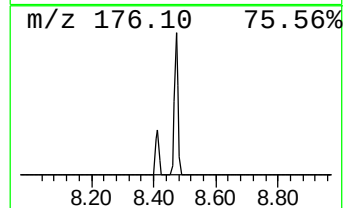
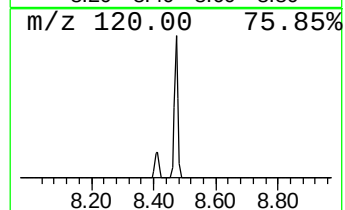
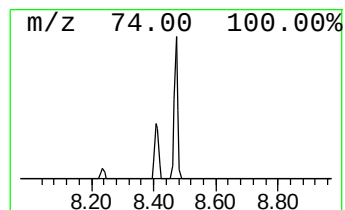
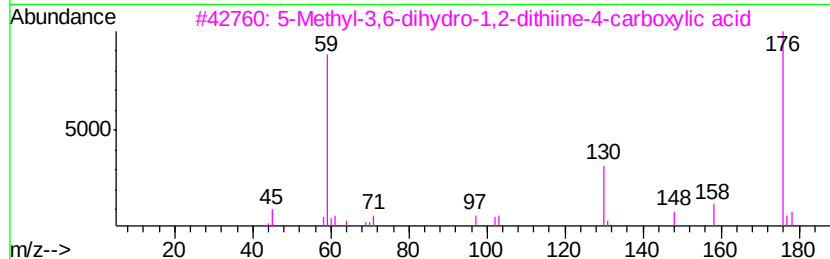
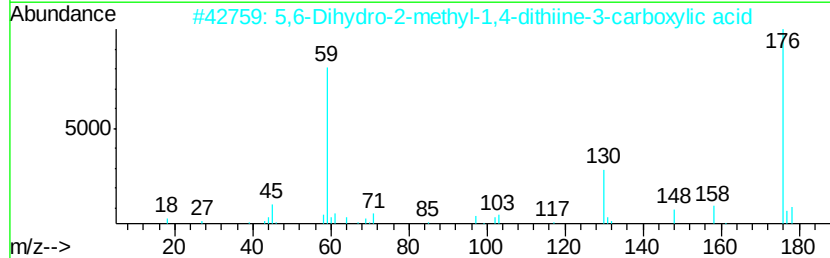
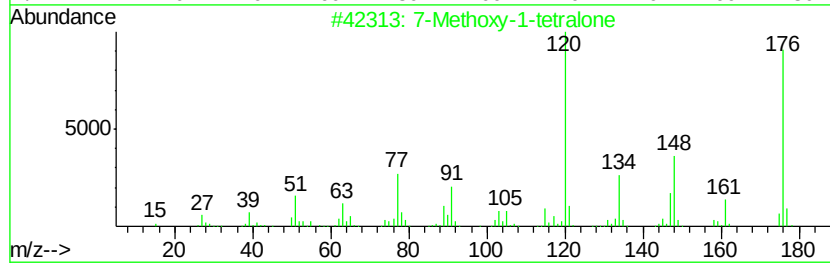
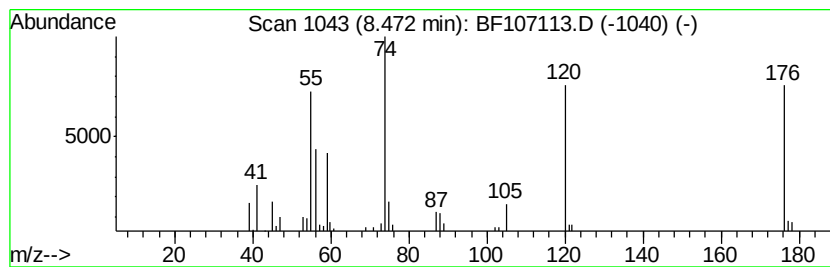
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Peak Number 4 unknown8.47 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.47	2.50 ng	41398	Napthalene-d8	8.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	7-Methoxy-1-tetralone	176	C11H12O2	006836-19-7	35
2		5,6-Dihydro-2-methyl-1,4-dithiin...	176	C6H8O2S2	035756-29-7	25
3		5-Methyl-3,6-dihydro-1,2-dithiin...	176	C6H8O2S2	959252-25-6	22
4		1,3-Dithiane	120	C4H8S2	000505-23-7	22
5		Phenylalanine	165	C9H11NO2	000063-91-2	17



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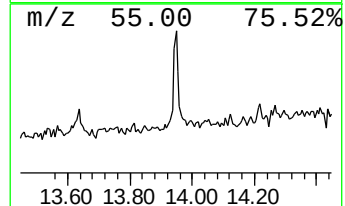
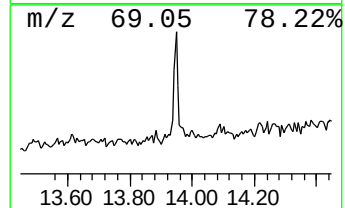
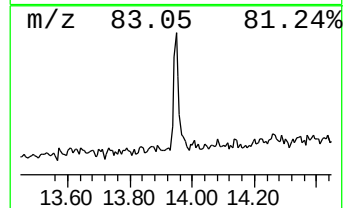
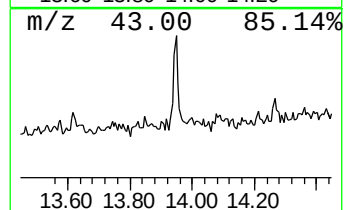
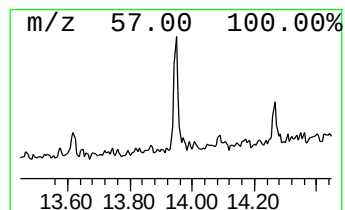
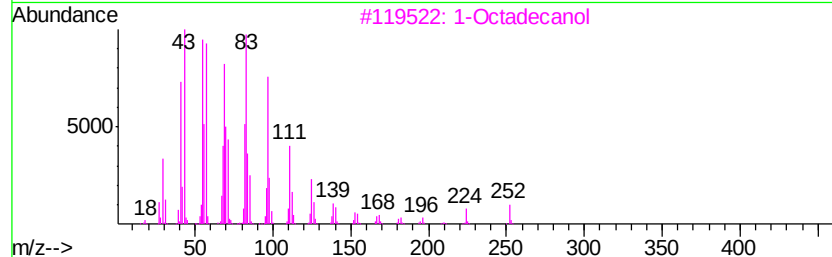
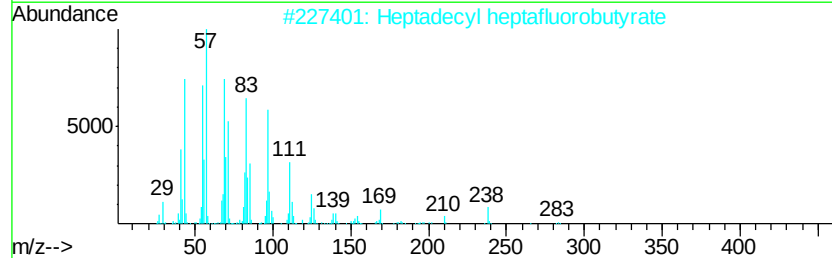
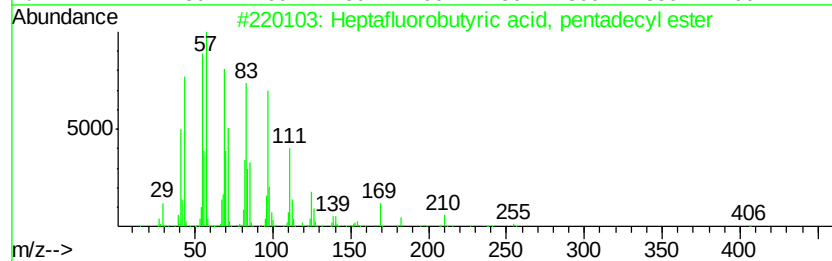
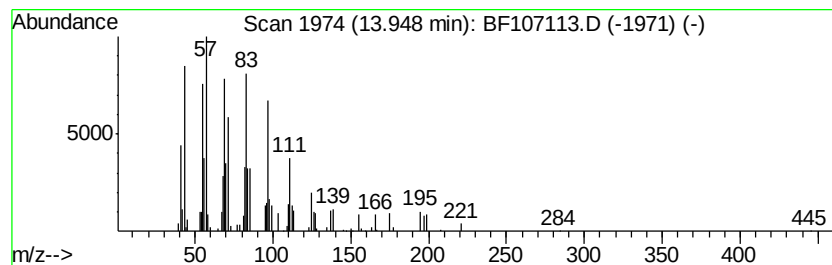
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Peak Number 5 Heptafluorobutyric acid, pe... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	2.58 ng	45592	Chrysene-d12	14.14

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	95
2		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3		1-Octadecanol	270	C18H38O	000112-92-5	93
4		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	92
5		Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	92



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetic acid, 1,1-...	5.18	3.5	ng	52603	1	6.95	304053	20.0
unknown6.74	6.74	71.8	ng	1092080	1	6.95	304053	20.0
unknown8.47	8.47	2.5	ng	41398	2	8.24	331751	20.0
Heptafluorobutyri...	13.95	2.6	ng	45592	5	14.14	353761	20.0