

Data Path : U:\HPCHEM1\BNA_F\DATA\BF011718\
 Data File : BF102180.D
 Acq On : 18 Jan 2018 5:56
 Operator : SJ/JU
 Sample : J1144-07
 Misc :
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DS-1

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-BF010918.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	4.940	480	485	497	rVB	187971	304229	7.52%	0.928%
2	5.334	547	552	555	rBV	3329917	3985885	98.55%	12.157%
3	6.363	720	727	731	rBV	3451399	4044403	100.00%	12.336%
4	6.492	743	749	752	rBV	4048152	4013960	99.25%	12.243%
5	6.716	784	787	791	rBV	965441	854046	21.12%	2.605%
6	6.875	809	814	817	rBV	3213114	3030881	74.94%	9.244%
7	7.286	878	884	887	rBV	2371017	2532252	62.61%	7.724%
8	7.998	1001	1005	1009	rBV	1257095	1113491	27.53%	3.396%
9	9.080	1183	1189	1192	rBV	4258028	3946796	97.59%	12.038%
10	9.469	1252	1255	1259	rBV	378492	322118	7.96%	0.982%
11	9.751	1295	1303	1307	rBV2	1260557	1141939	28.24%	3.483%
12	10.469	1420	1425	1428	rBV	76790	68270	1.69%	0.208%
13	10.539	1432	1437	1441	rBV	2067780	2136217	52.82%	6.516%
14	11.233	1551	1555	1559	rBV	1128555	928411	22.96%	2.832%
15	12.645	1792	1795	1798	rVB	80446	64284	1.59%	0.196%
16	12.704	1800	1805	1807	rBV	93640	127821	3.16%	0.390%
17	12.821	1820	1825	1828	rBV	2709261	2475276	61.20%	7.550%
18	13.710	1973	1976	1984	rBV	346756	324093	8.01%	0.989%
19	13.862	1998	2002	2006	rBV	695784	672173	16.62%	2.050%
20	15.280	2238	2243	2247	rBV	561523	649468	16.06%	1.981%
21	15.768	2324	2326	2331	rVB4	41711	49903	1.23%	0.152%

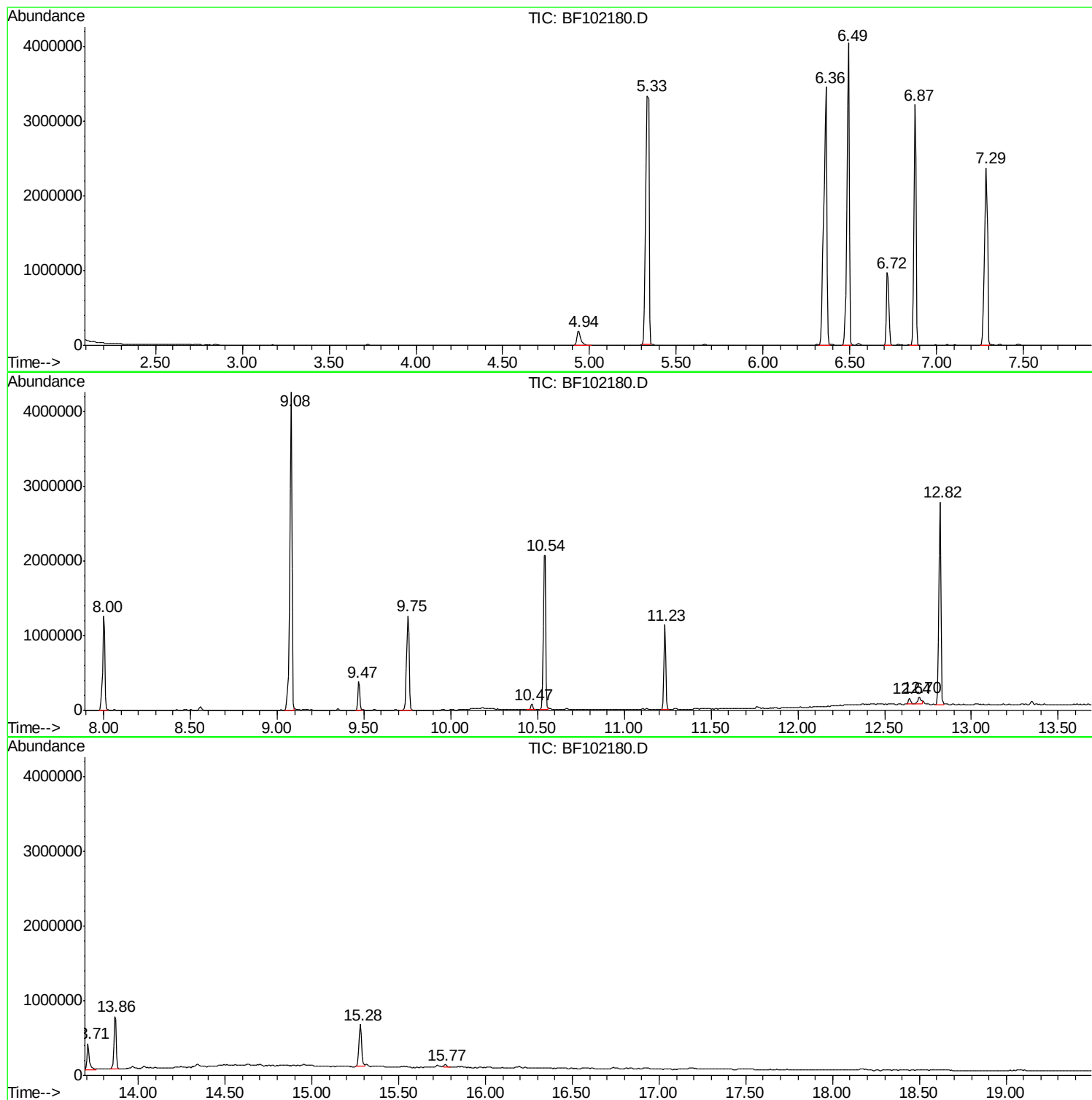
Sum of corrected areas: 32785916

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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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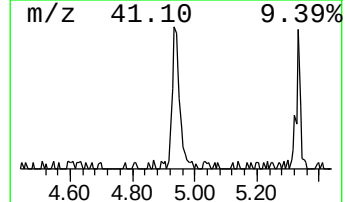
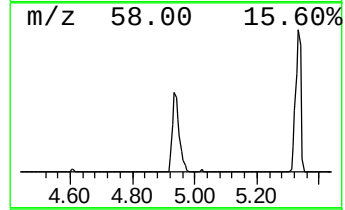
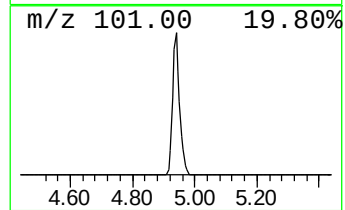
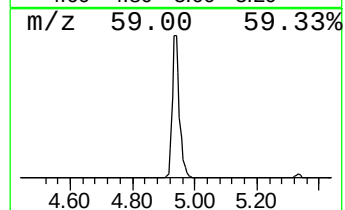
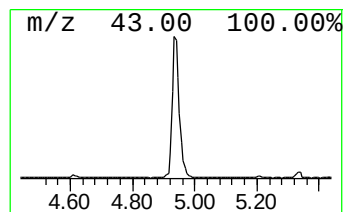
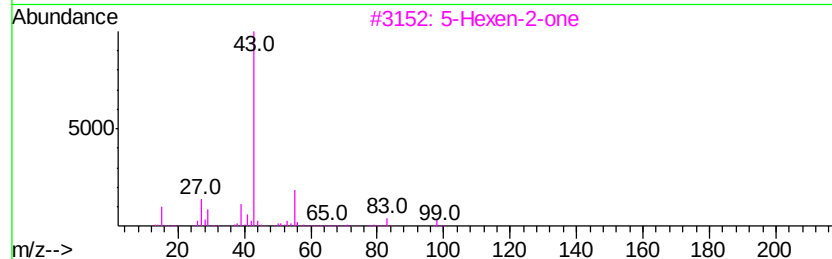
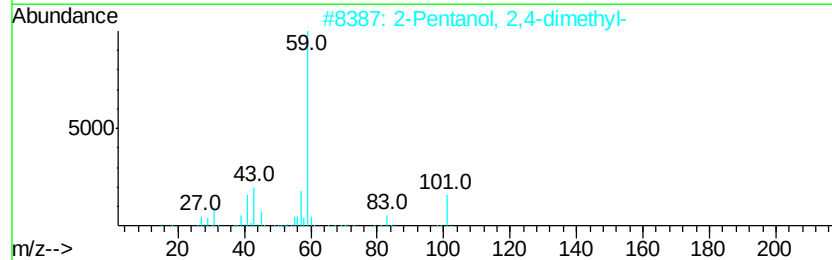
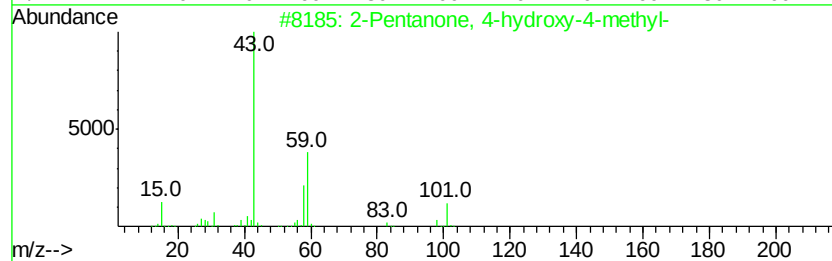
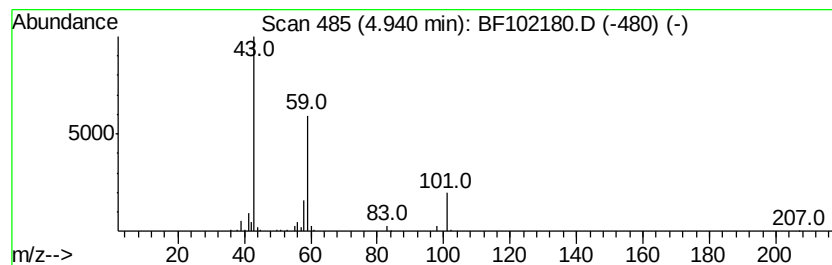
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.94	7.12 ng	304229	1,4-Dichlorobenzene-d4	6.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	25
3			5-Hexen-2-one	98	C6H10O	000109-49-9	9
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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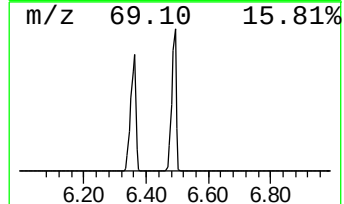
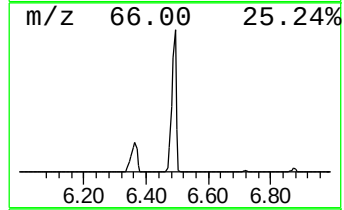
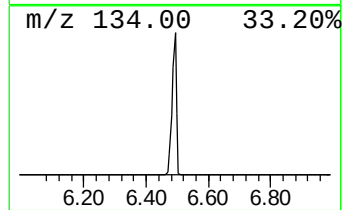
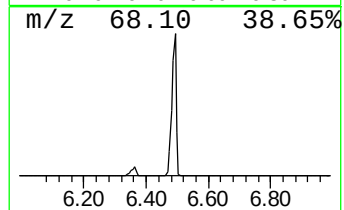
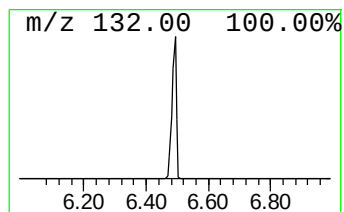
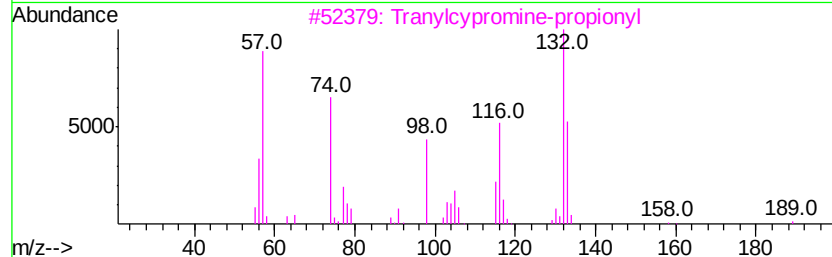
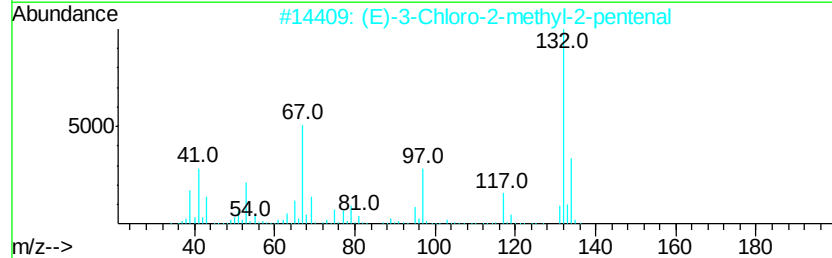
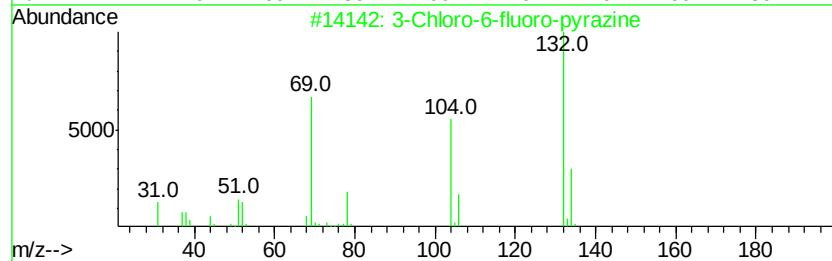
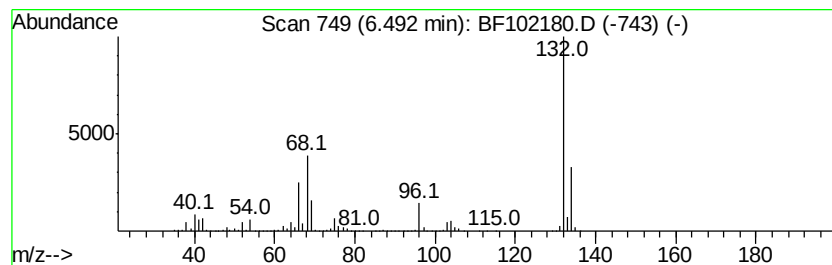
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Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	94.00 ng	4013960	1,4-Dichlorobenzene-d4	6.72

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		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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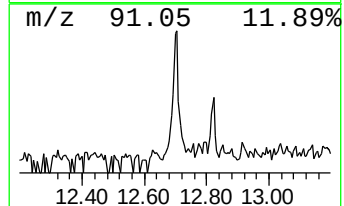
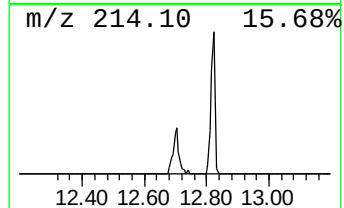
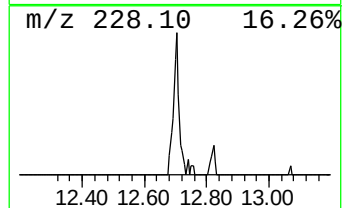
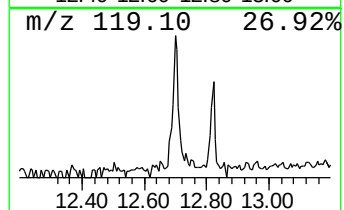
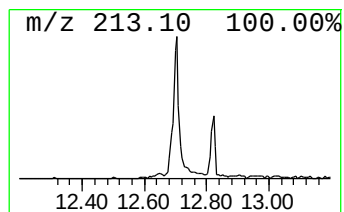
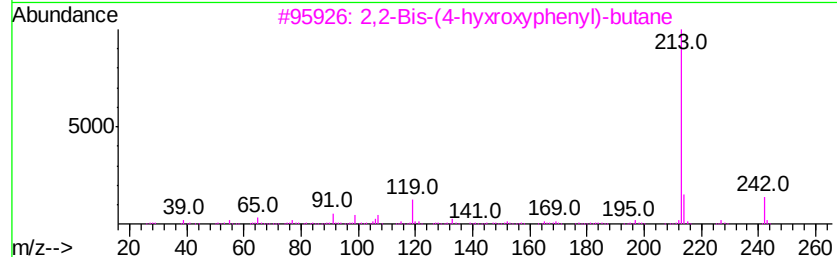
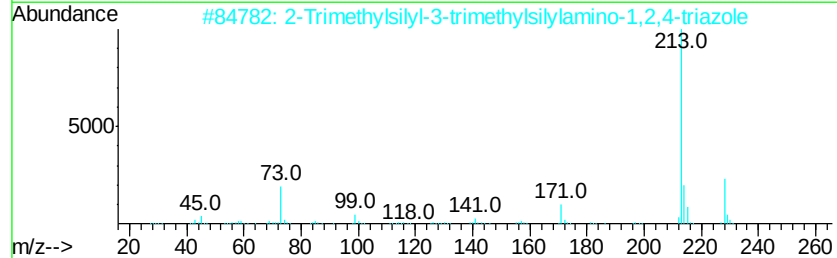
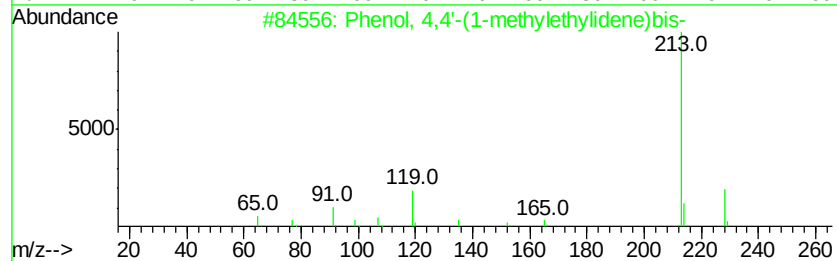
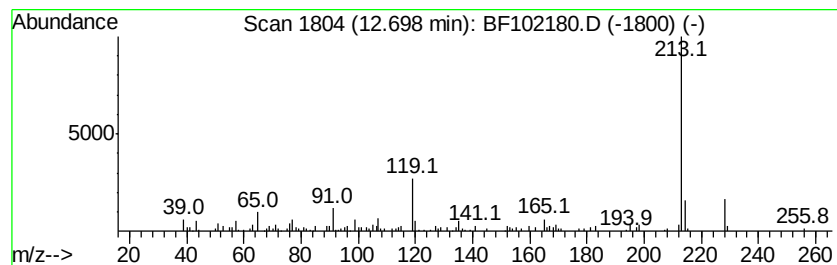
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Peak Number 4 Phenol, 4,4'-(1-methylethyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.70	3.80 ng	127821	Chrysene-d12	13.86	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene)bis-	228	C15H16O2	000080-05-7	97
2	2-Trimethylsilyl-3-trimethylsilyl-	228	C8H20N4Si2	1000373-05-5	70
3	2,2-Bis-(4-hydroxyphenyl)-butane	242	C16H18O2	000077-40-7	59
4	2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	58
5	2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	50



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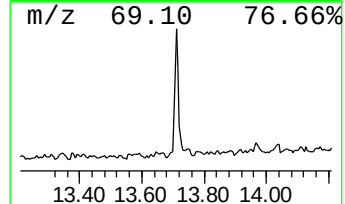
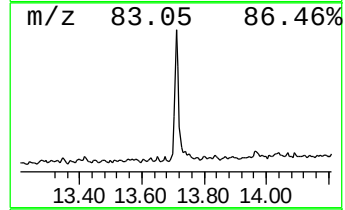
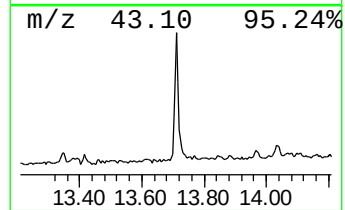
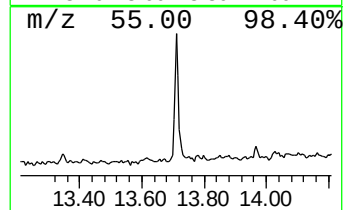
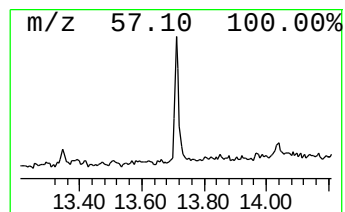
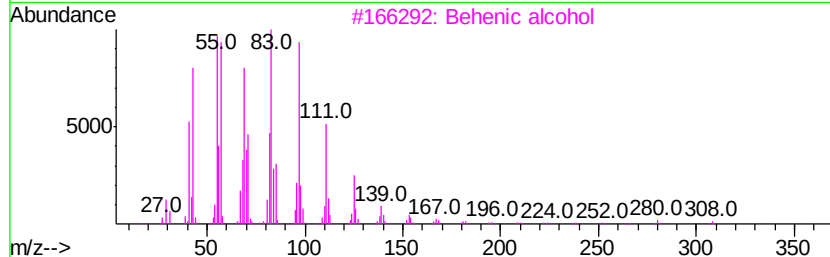
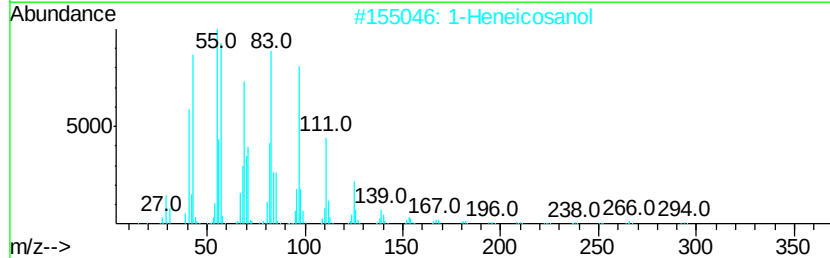
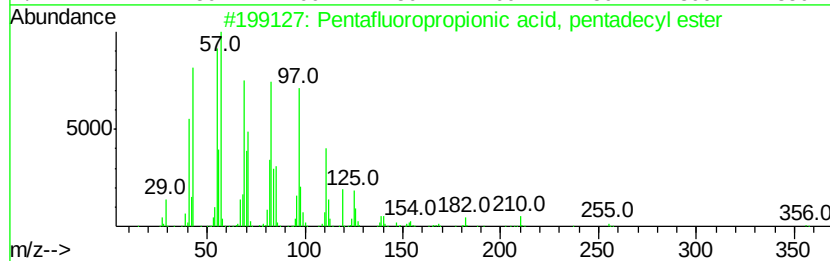
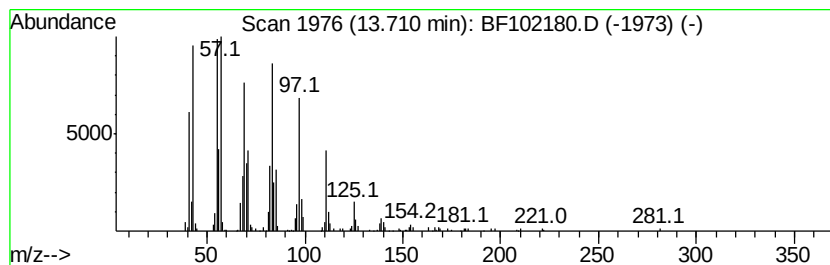
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Peak Number 5 Pentafluoropropionic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	9.64 ng	324093	Chrysene-d12	13.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
2		1-Heneicosanol	312	C21H44O	015594-90-8	94
3		Behenic alcohol	326	C22H46O	000661-19-8	91
4		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
5		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.94	7.1	ng	304229	1	6.72	854046	20.0
unknown6.49	6.49	94.0	ng	4013960	1	6.72	854046	20.0
Phenol, 4,4'-(1-m...	12.70	3.8	ng	127821	5	13.86	672173	20.0
Pentafluoropropio...	13.71	9.6	ng	324093	5	13.86	672173	20.0