

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012023\
 Data File : BF132180.D
 Acq On : 21 Jan 2023 01:28
 Operator : CG\JU
 Sample : 01233-05
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-P36B

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-BF011923.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132180.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.748	321	325	331	rVB	109623	115974	2.68%	0.375%
2	5.337	419	425	435	rVB	1623943	1992472	46.03%	6.439%
3	5.713	484	489	492	rBV	3536104	3388532	78.28%	10.951%
4	6.337	592	595	601	rVB	43664	52863	1.22%	0.171%
5	6.701	651	657	660	rBV	3214803	3757902	86.82%	12.144%
6	7.090	719	723	726	rBV	1314430	1077976	24.90%	3.484%
7	7.648	813	818	821	rBV	2730066	2471515	57.10%	7.987%
8	8.372	938	941	945	rVB	1500925	1343099	31.03%	4.340%
9	9.454	1120	1125	1128	rBV	4335422	4134281	95.51%	13.361%
10	10.136	1238	1241	1245	rBV	1656645	1535169	35.47%	4.961%
11	10.854	1359	1363	1366	rBV	261916	206428	4.77%	0.667%
12	10.930	1372	1376	1379	rBV	2737317	2313946	53.46%	7.478%
13	11.636	1492	1496	1500	rBV	1866321	1610864	37.21%	5.206%
14	11.701	1504	1507	1510	rVB	108625	85028	1.96%	0.275%
15	12.142	1577	1582	1588	rBV	156516	136744	3.16%	0.442%
16	13.230	1763	1767	1771	rBV	4456950	4328627	100.00%	13.989%
17	14.124	1916	1919	1927	rBV	80775	155258	3.59%	0.502%
18	14.301	1945	1949	1952	rBV	1274477	1196032	27.63%	3.865%
19	15.895	2214	2220	2236	rVB	761300	1040982	24.05%	3.364%

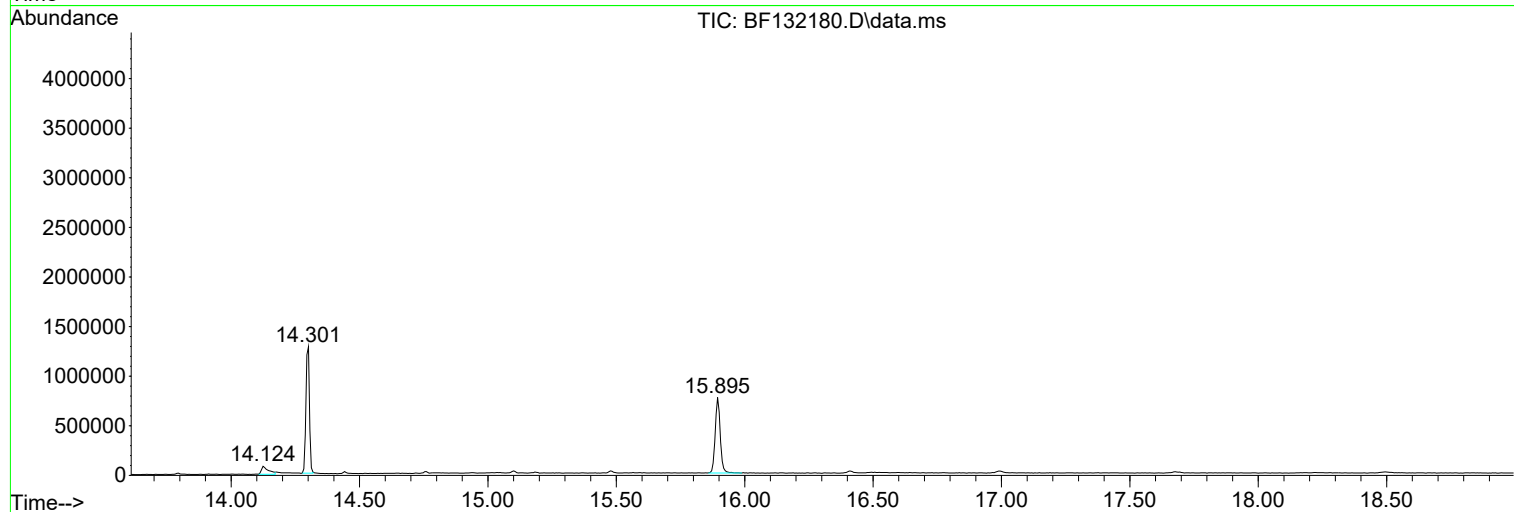
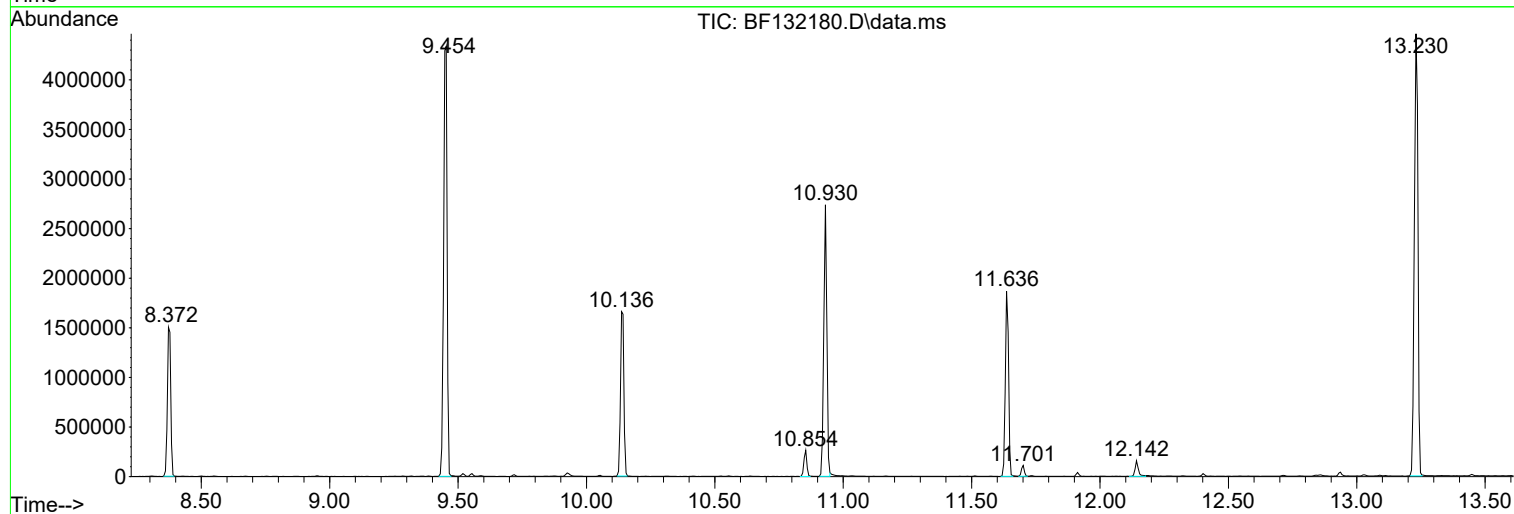
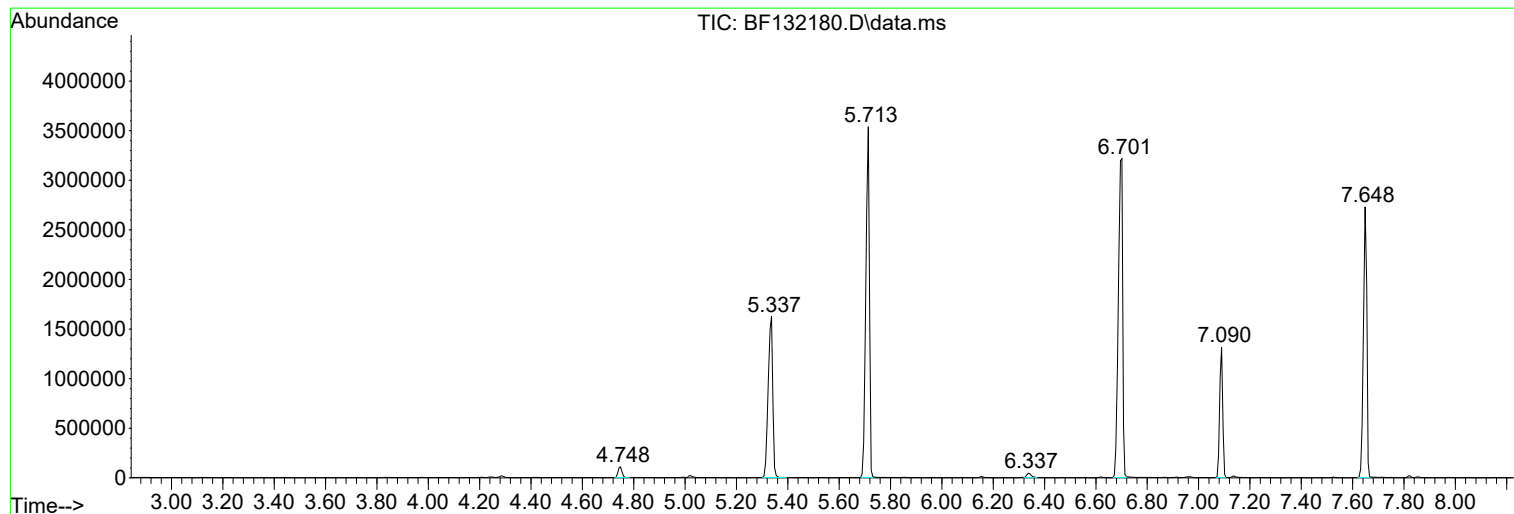
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011923.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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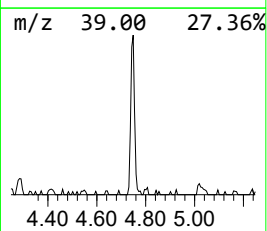
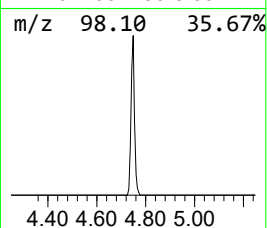
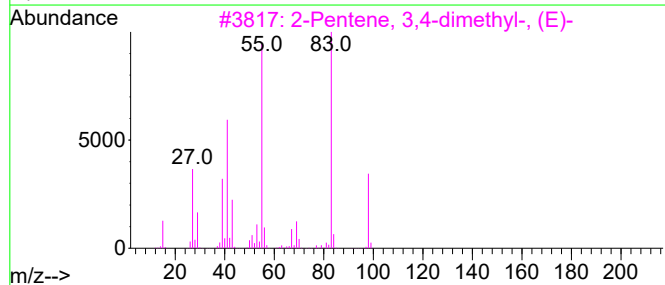
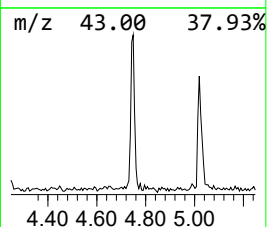
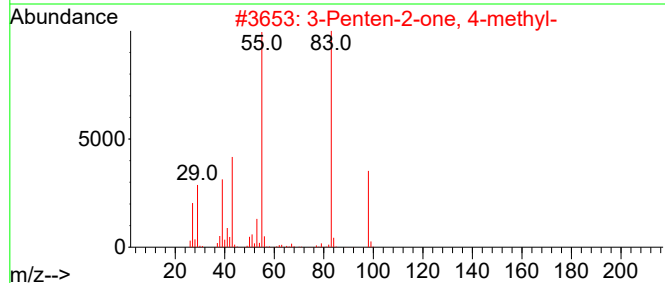
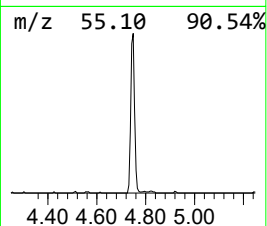
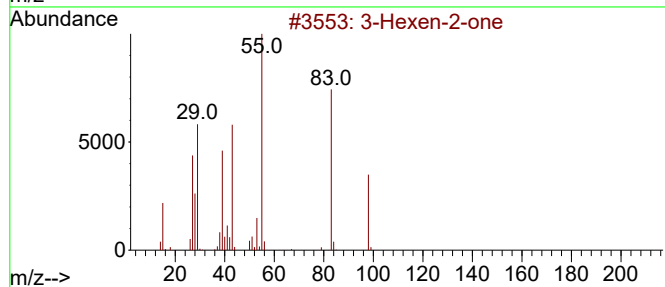
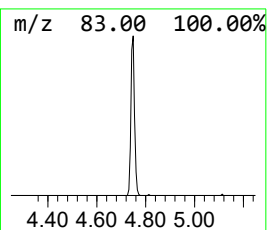
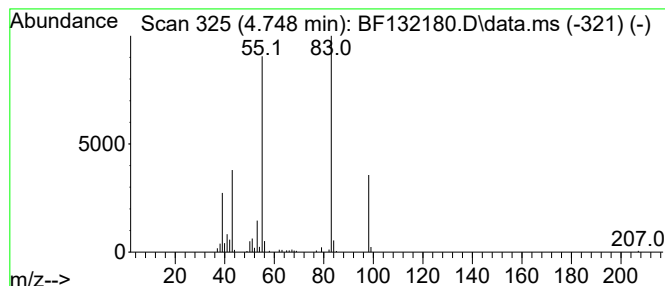
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Hexen-2-one Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.748	2.15 ng	115974	1,4-Dichlorobenzene-d4	7.090

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexen-2-one	98	C6H10O	000763-93-9	91
2			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80



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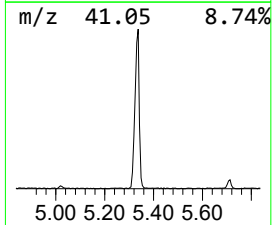
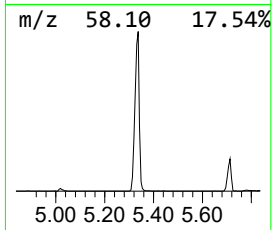
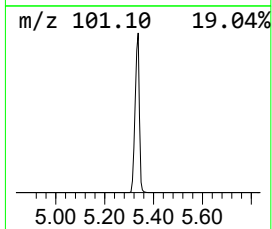
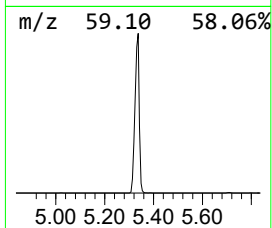
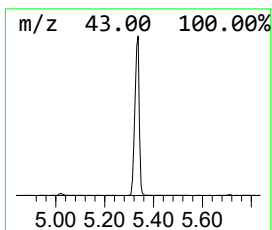
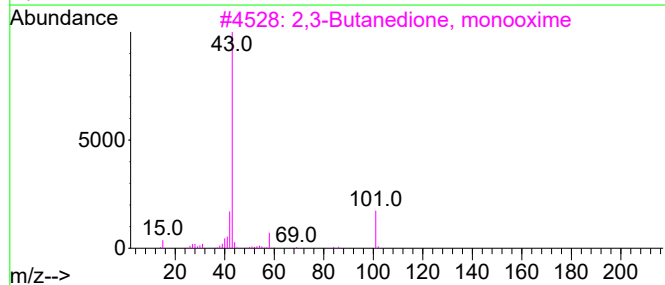
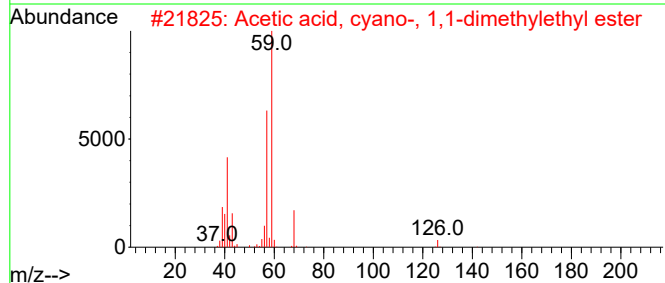
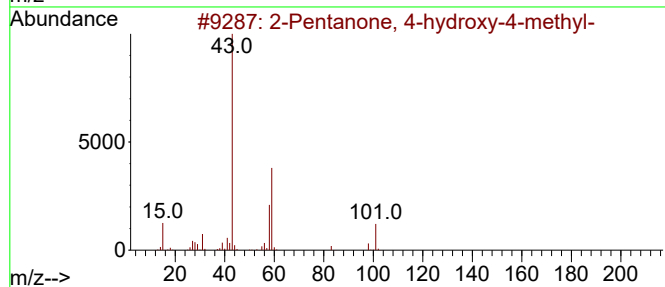
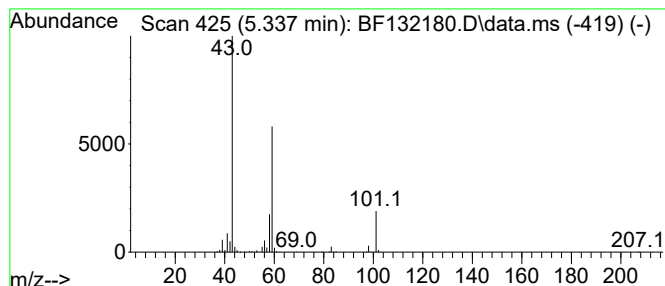
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011923.M
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.337	36.97 ng	1992470	1,4-Dichlorobenzene-d4	7.090

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			Acetone	58	C3H6O	000067-64-1	10



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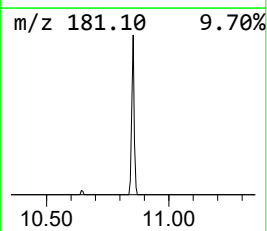
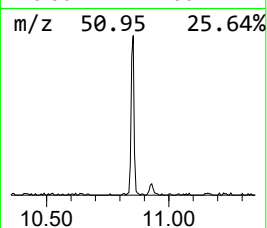
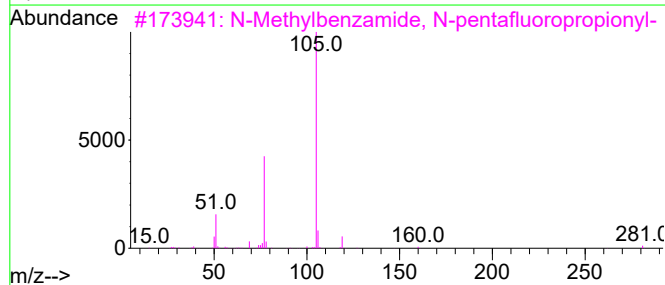
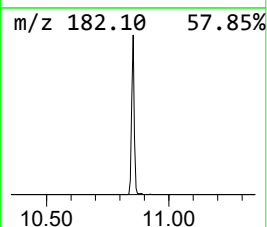
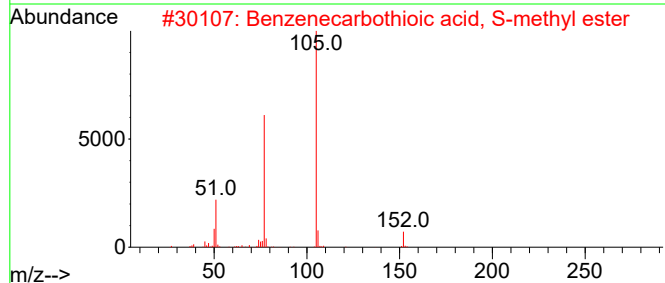
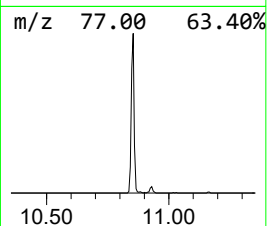
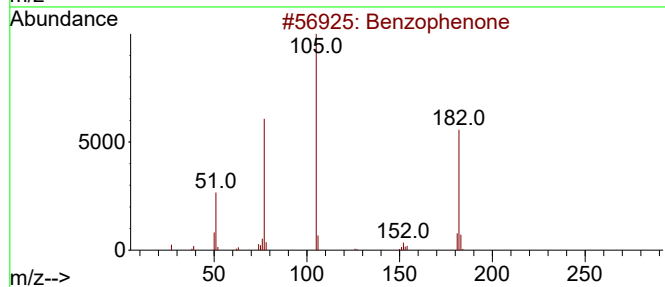
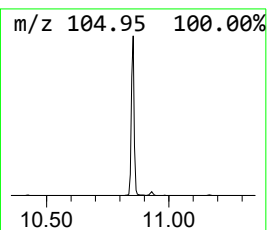
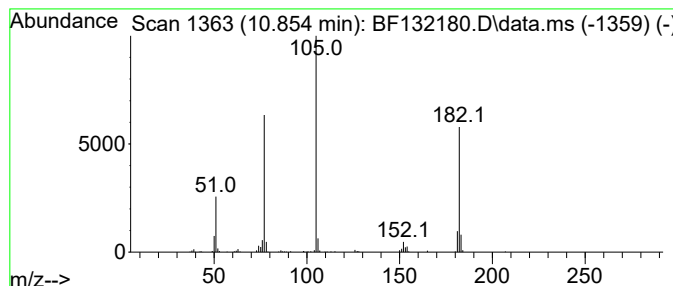
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Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.854	2.69 ng	206428	Acenaphthene-d10	10.142

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	49
3			N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	47
4			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
5			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47



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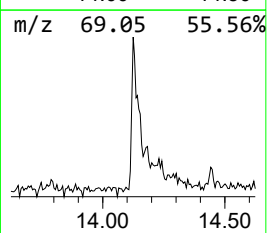
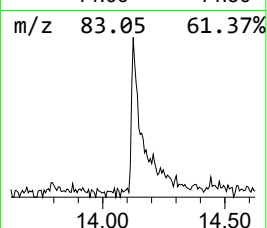
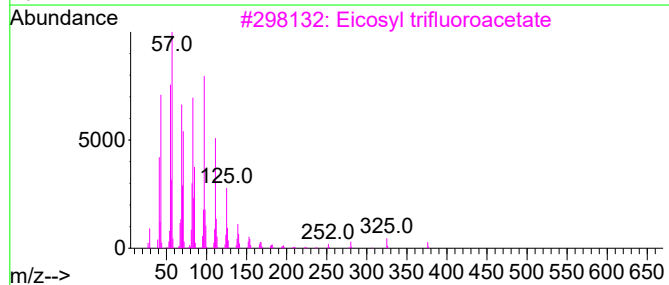
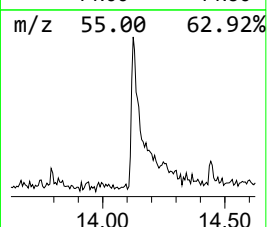
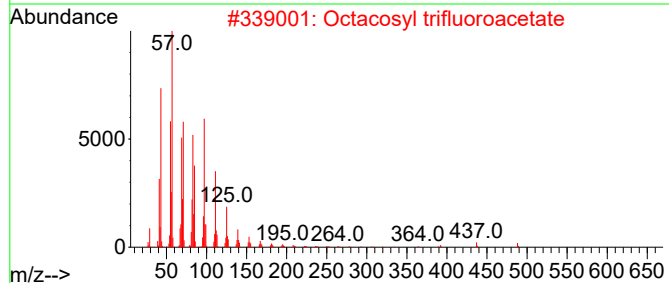
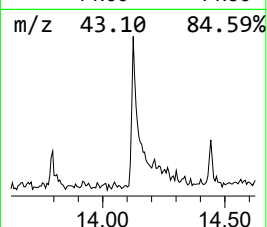
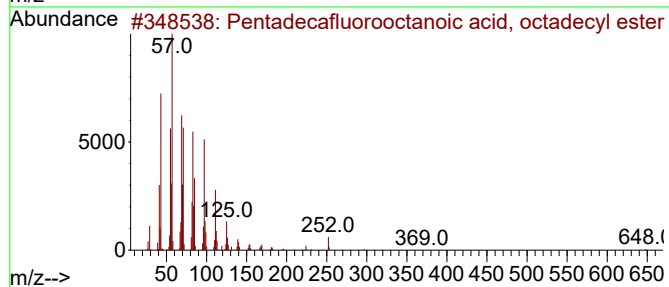
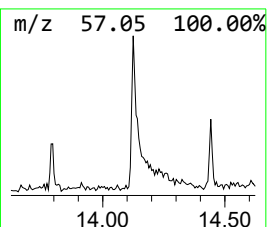
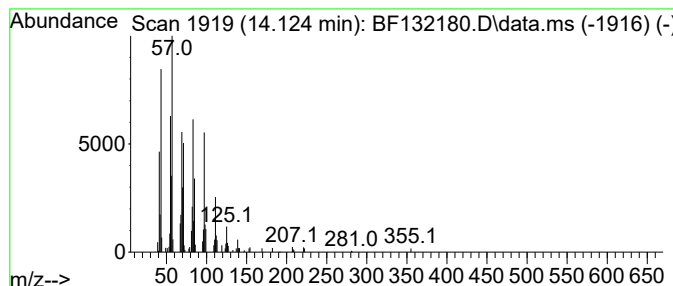
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Peak Number 4 Pentadecafluorooctanoic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.124	2.60 ng	155258	Chrysene-d12	14.301

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
3			Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	91
4			1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91
5			Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Hexen-2-one	4.748	2.1	ng	115974	1	7.090	1077980	20.0
2-Pentanone, 4-...	5.337	37.0	ng	1992470	1	7.090	1077980	20.0
Benzophenone	10.854	2.7	ng	206428	3	10.142	1535170	20.0
Pentadecafluoro...	14.124	2.6	ng	155258	5	14.301	1196030	20.0