

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101723\
 Data File : BF135821.D
 Acq On : 17 Oct 2023 19:59
 Operator : CG\JU
 Sample : 04723-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-4B

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-BF101323.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135821.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.340	380	383	392	rBV2	17863	37520	1.13%	0.215%
2	4.952	484	487	505	rBV	407689	505448	15.21%	2.893%
3	5.375	556	559	583	rBV	929716	1210175	36.41%	6.927%
4	5.757	621	624	632	rBV	43350	46668	1.40%	0.267%
5	6.393	729	732	758	rBV	466445	680949	20.49%	3.898%
6	6.734	787	790	801	rBV	622330	563070	16.94%	3.223%
7	7.310	884	888	902	rBV	2014078	2005660	60.35%	11.481%
8	8.016	1005	1008	1023	rBV	874044	760545	22.88%	4.354%
9	9.098	1188	1192	1195	rBV	3772612	3323425	100.00%	19.024%
10	9.775	1303	1307	1321	rVB	973917	863175	25.97%	4.941%
11	10.575	1439	1443	1457	rBV	2141859	2086208	62.77%	11.942%
12	10.698	1461	1464	1473	rVB	71998	87331	2.63%	0.500%
13	11.269	1558	1561	1571	rBV	983309	852905	25.66%	4.882%
14	11.804	1648	1652	1668	rBV2	108599	163833	4.93%	0.938%
15	12.592	1783	1786	1800	rBV	33346	56270	1.69%	0.322%
16	12.869	1828	1833	1836	rBV	3163337	3061697	92.12%	17.526%
17	13.845	1993	1999	2006	rBV8	21366	58741	1.77%	0.336%
18	13.933	2011	2014	2024	rVV	600102	584542	17.59%	3.346%
19	15.410	2261	2265	2278	rBV	367564	521098	15.68%	2.983%

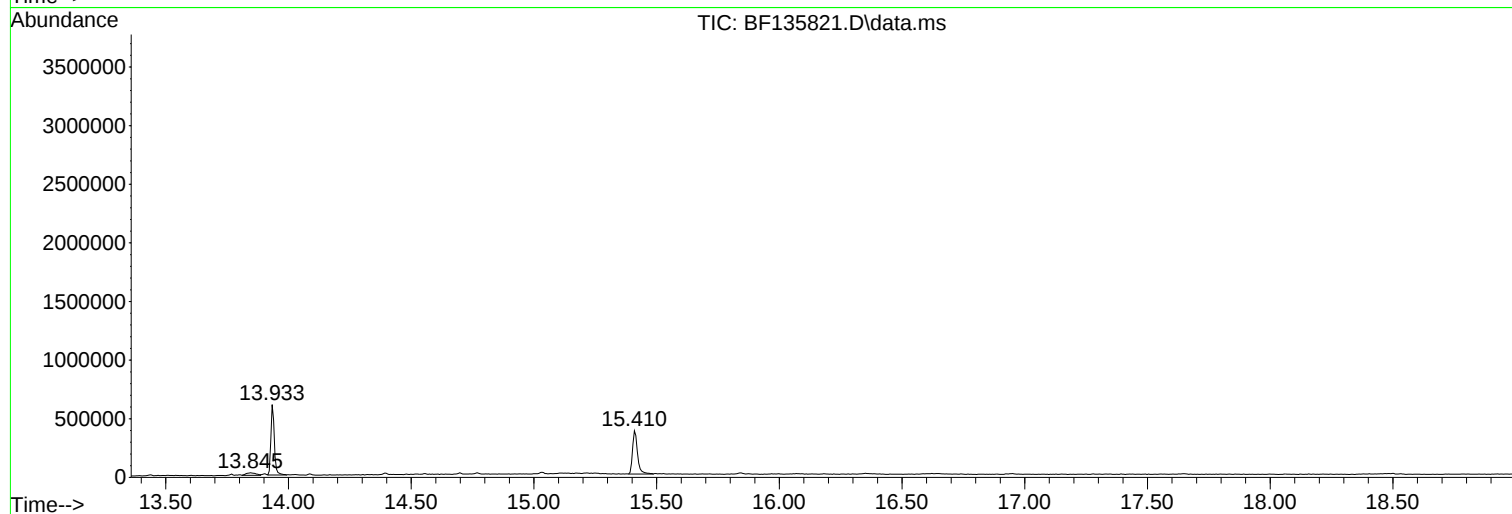
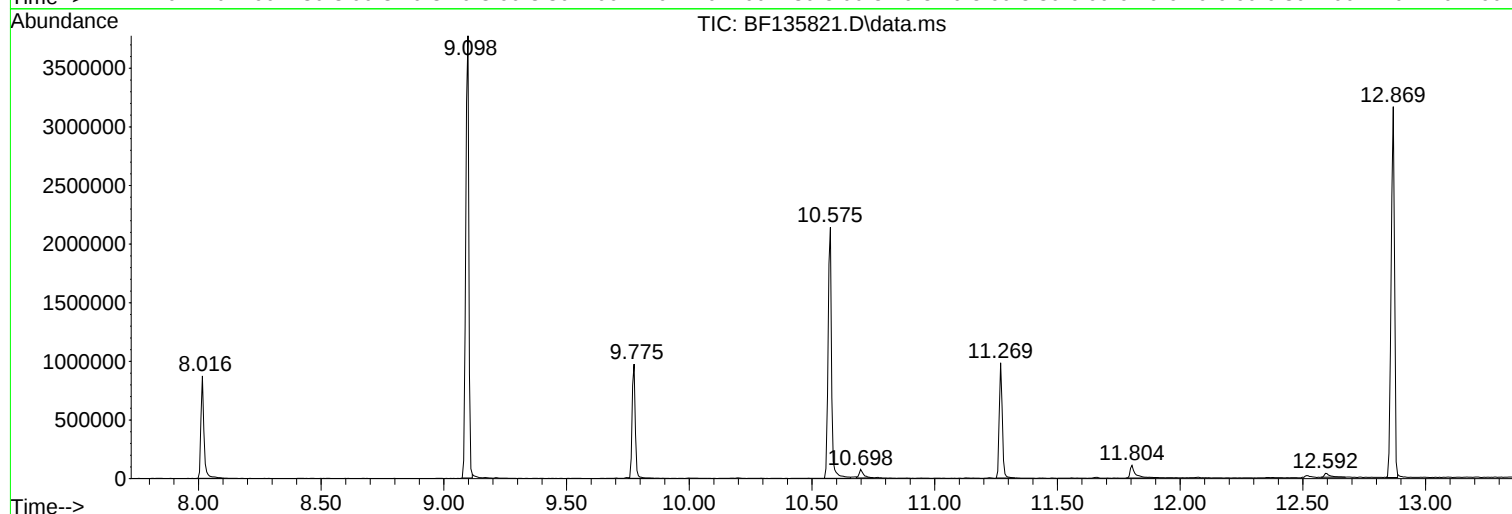
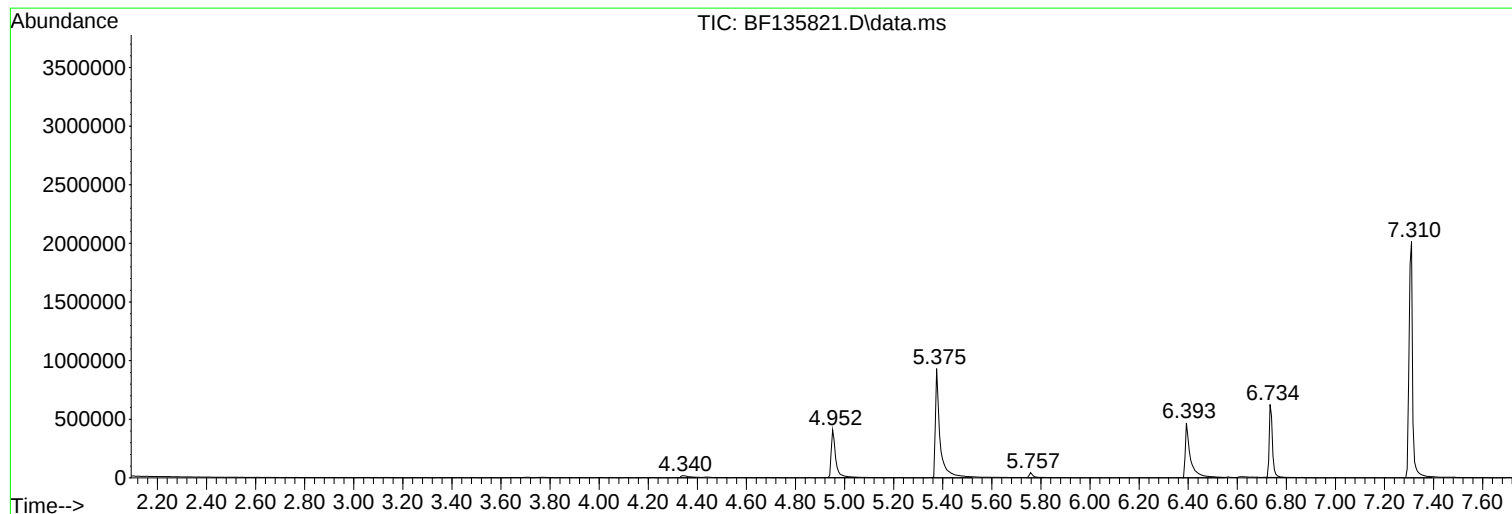
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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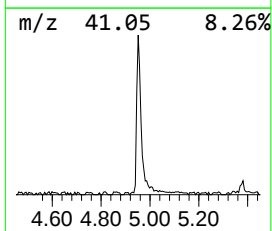
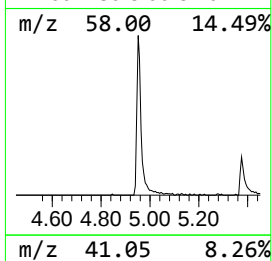
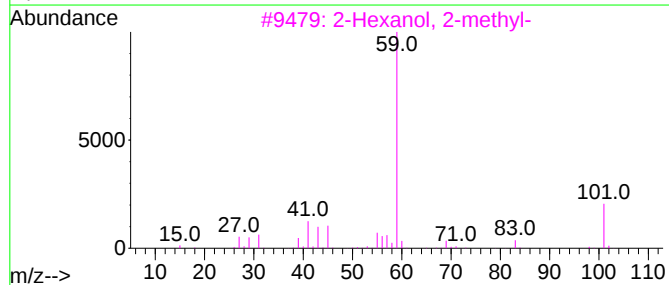
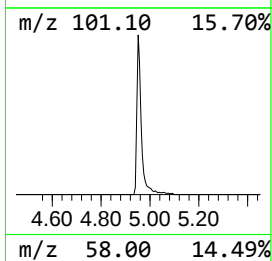
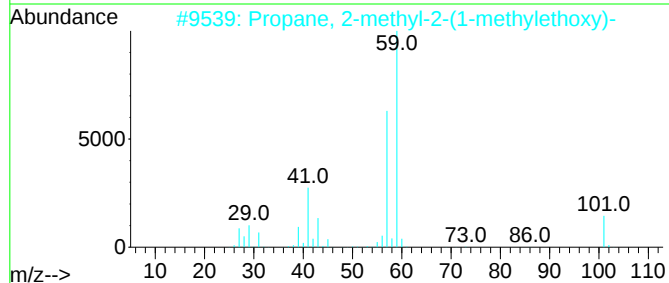
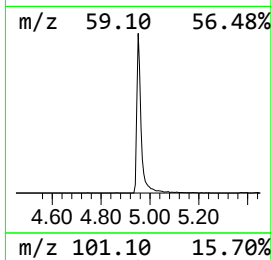
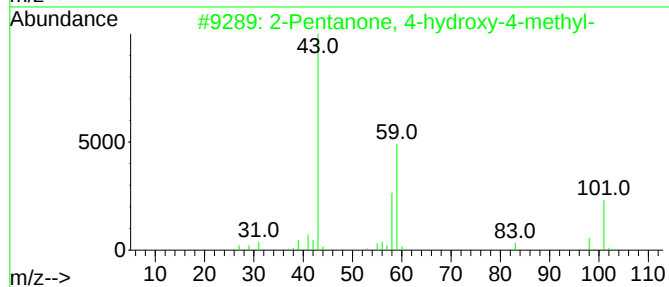
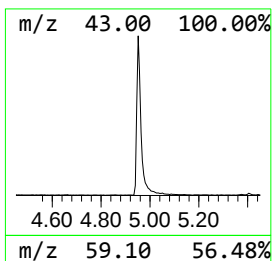
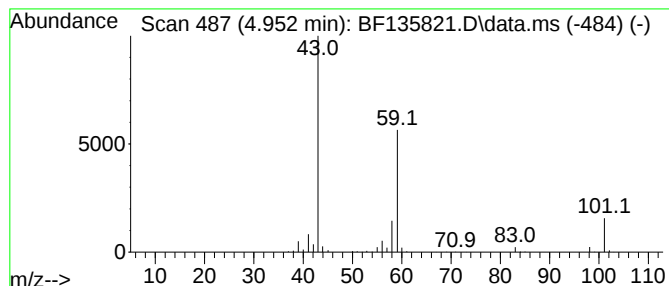
Instrument :
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ClientSampleId :
MW-4B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
4.952	17.95 ng	505448	1,4-Dichlorobenzene-d4			6.734
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	53
2	Propane, 2-methyl-2-(1-methyleth...		116	C7H16O	017348-59-3	42
3	2-Hexanol, 2-methyl-		116	C7H16O	000625-23-0	33
4	3-Hexanol		102	C6H14O	000623-37-0	33
5	3-Hexanol, 4-methyl-		116	C7H16O	000615-29-2	33



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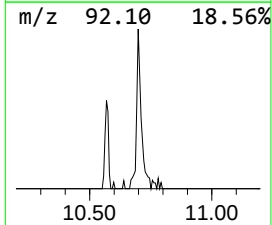
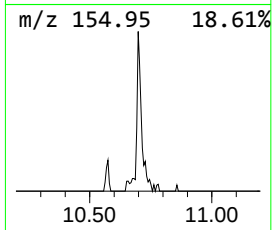
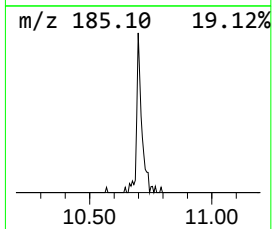
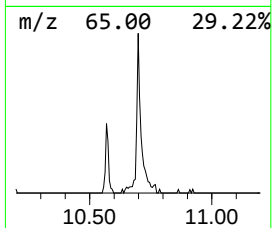
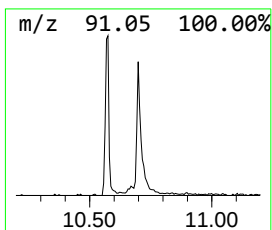
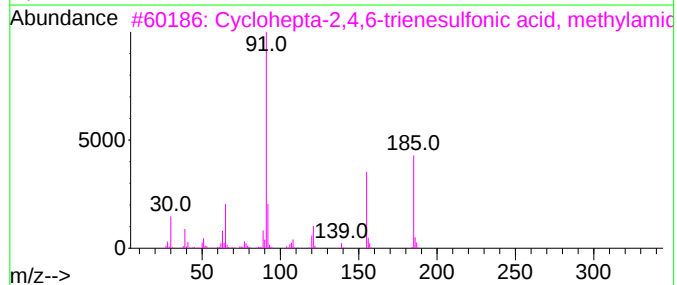
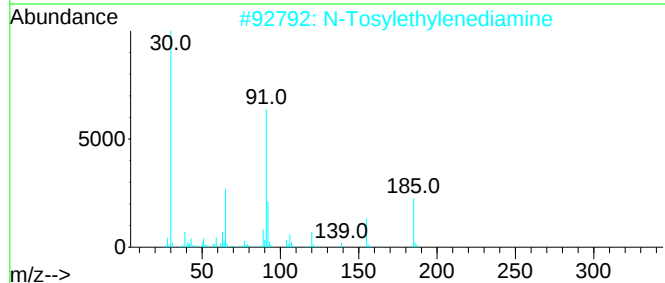
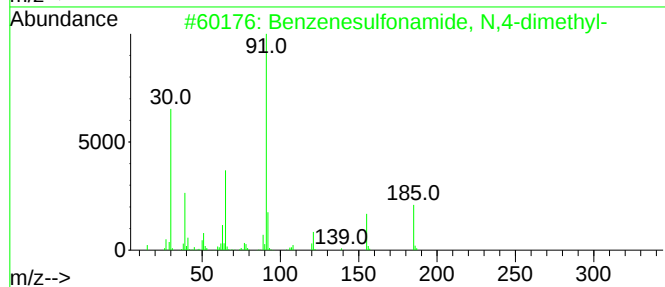
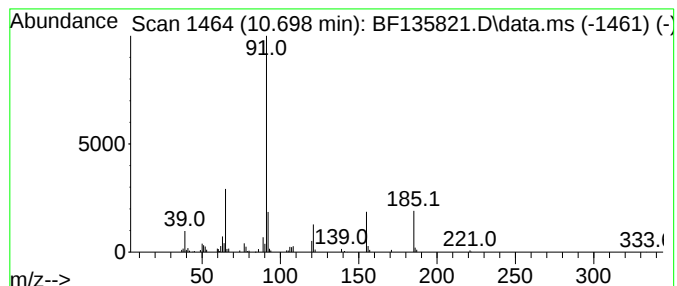
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Peak Number 2 Benzenesulfonamide, N,4-dim... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.698	2.05 ng	87331	Phenanthrene-d10	11.269	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	95
2	N-Tosylethylenediamine	214	C9H14N2O2S	014316-16-6	59
3	Cyclohepta-2,4,6-trienesulfonic ...	185	C8H11NO2S	1000187-28-7	52
4	Ethyl(E/Z)-.alpha.-cyano-4-nitro...	416	C19H16N2O7S	1000287-26-8	50
5	N-Sulfinyl-p-toluenesulfonamide	217	C7H7NO3S2	004104-47-6	47



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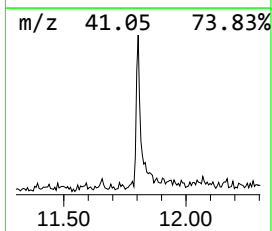
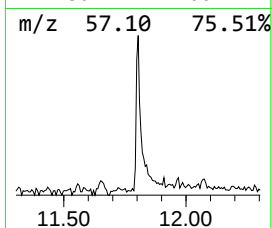
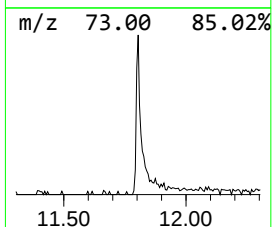
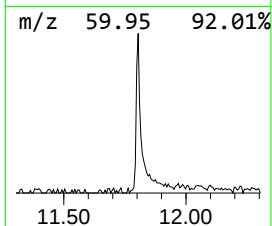
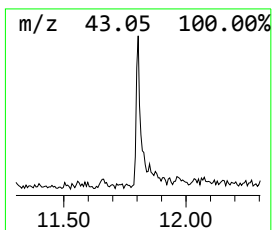
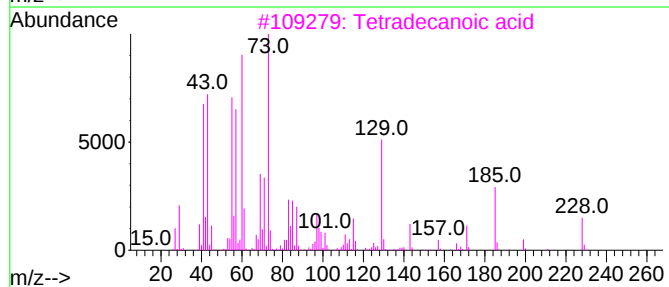
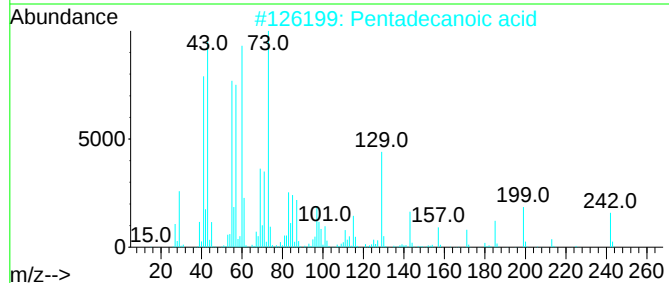
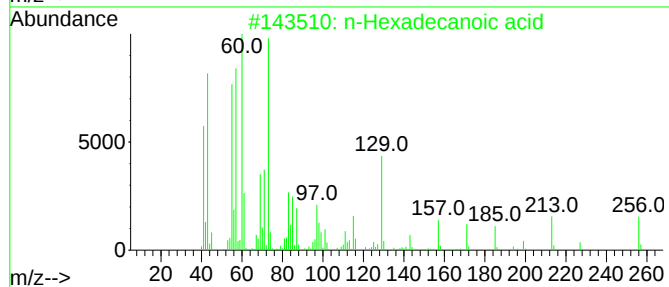
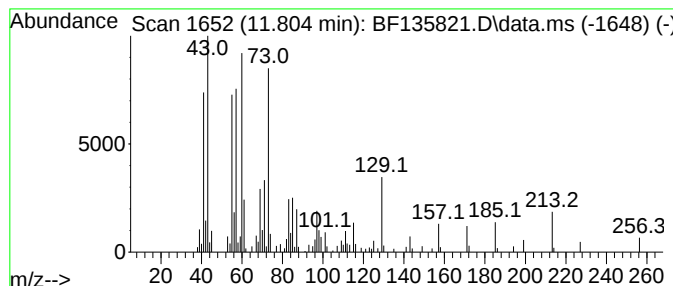
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	3.84 ng	163833	Phenanthrene-d10	11.269

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4		n-Decanoic acid	172	C10H20O2	000334-48-5	83
5		Tridecanoic acid	214	C13H26O2	000638-53-9	59



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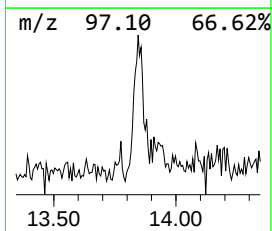
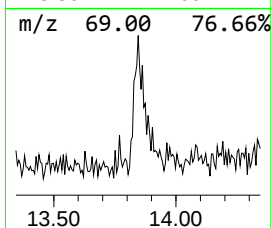
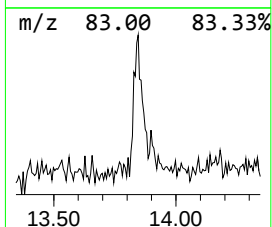
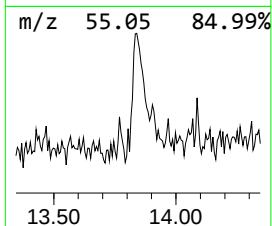
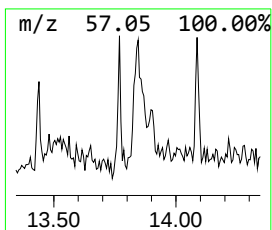
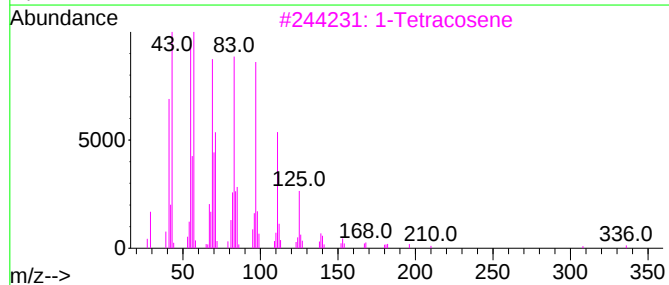
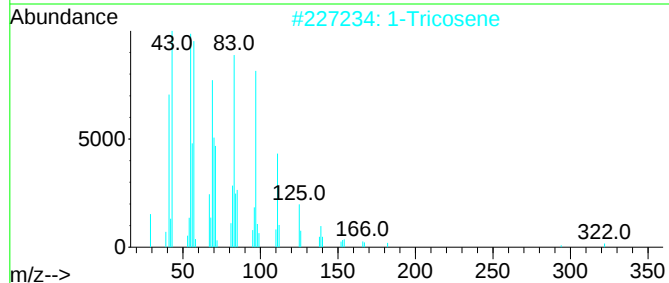
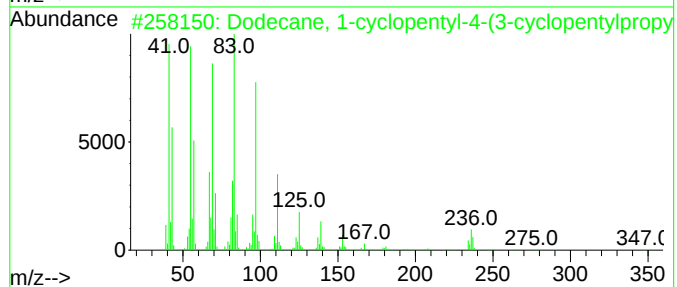
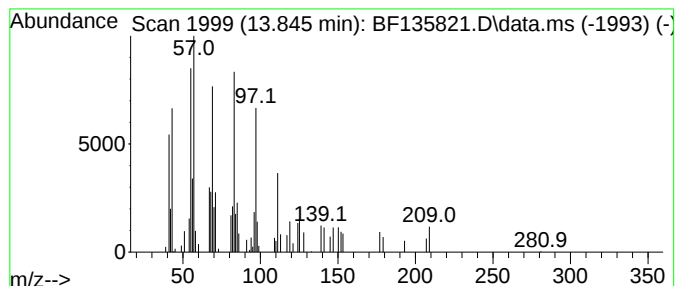
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Peak Number 4 Dodecane, 1-cyclopentyl-4-(... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.845	2.01 ng	58741	Chrysene-d12	13.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 1-cyclopentyl-4-(3-cyc...	348	C25H48	007225-68-5	72
2			1-Tricosene	322	C23H46	018835-32-0	72
3			1-Tetracosene	336	C24H48	010192-32-2	72
4			Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	72
5			Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	000547-60-4	49



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.952	17.9	ng	505448	1	6.734	563070	20.0
Benzenesulfonam...	10.698	2.0	ng	87331	4	11.269	852905	20.0
n-Hexadecanoic ...	11.804	3.8	ng	163833	4	11.269	852905	20.0
Dodecane, 1-cyc...	13.845	2.0	ng	58741	5	13.933	584542	20.0