

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092223\
 Data File : BF135410.D
 Acq On : 22 Sep 2023 20:43
 Operator : CG\JU
 Sample : 04436-12
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B102-11

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-BF091123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135410.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	7	12	rBV	44422	68064	2.35%	0.316%
2	4.987	490	493	501	rBV	168652	218291	7.54%	1.013%
3	5.393	558	562	580	rBV	2857464	2896304	100.00%	13.439%
4	6.404	730	734	750	rBV	2855614	2848125	98.34%	13.215%
5	6.593	762	766	771	rBV2	36527	44253	1.53%	0.205%
6	6.757	791	794	802	rVB	1276710	999592	34.51%	4.638%
7	7.322	886	890	893	rBV	2045001	1776986	61.35%	8.245%
8	8.034	1008	1011	1015	rBV	1391808	1251640	43.22%	5.807%
9	9.116	1190	1195	1198	rBV	2935562	2635123	90.98%	12.227%
10	9.234	1211	1215	1220	rBV2	33272	49701	1.72%	0.231%
11	9.792	1306	1310	1327	rVB	1480214	1292885	44.64%	5.999%
12	10.586	1441	1445	1455	rBV	1647730	1525647	52.68%	7.079%
13	11.286	1560	1564	1570	rBV	1336970	1154481	39.86%	5.357%
14	11.822	1651	1655	1663	rBV	297424	332482	11.48%	1.543%
15	12.610	1786	1789	1794	rBV6	65072	106143	3.66%	0.492%
16	12.880	1831	1835	1839	rBV	1840322	1570594	54.23%	7.287%
17	13.369	1913	1918	1923	rBV	437553	520217	17.96%	2.414%
18	13.863	1995	2002	2003	rBV6	170453	351255	12.13%	1.630%
19	13.945	2012	2016	2024	rVB	880171	1062765	36.69%	4.931%
20	15.410	2261	2265	2269	rBV	661315	847710	29.27%	3.933%

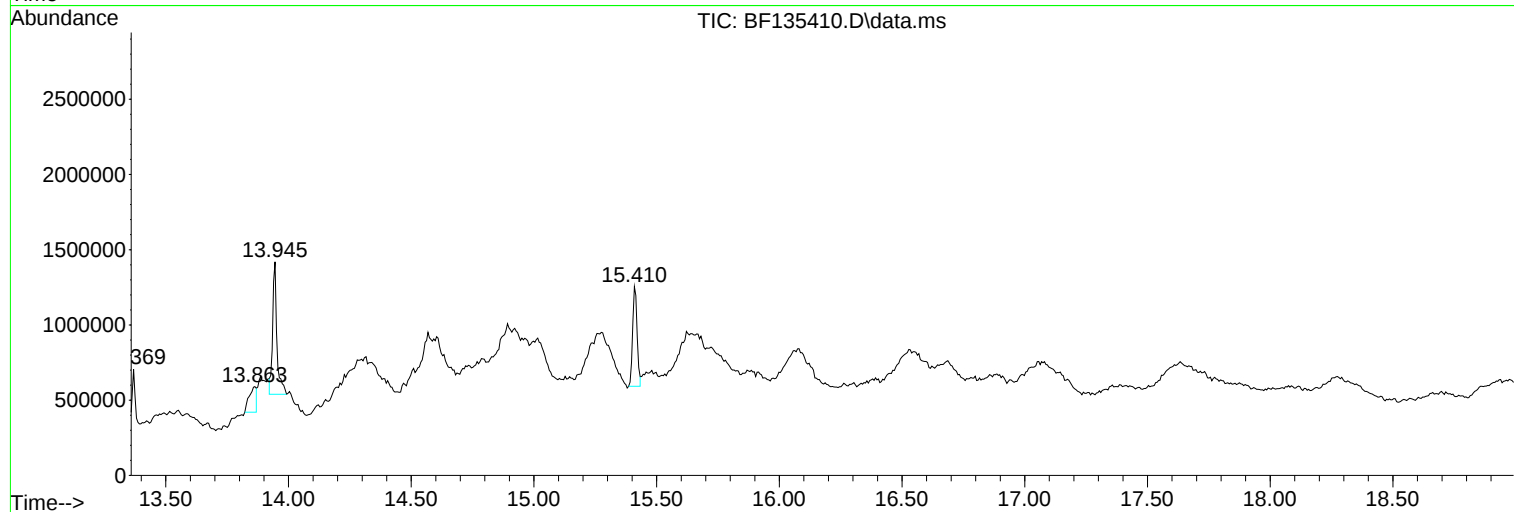
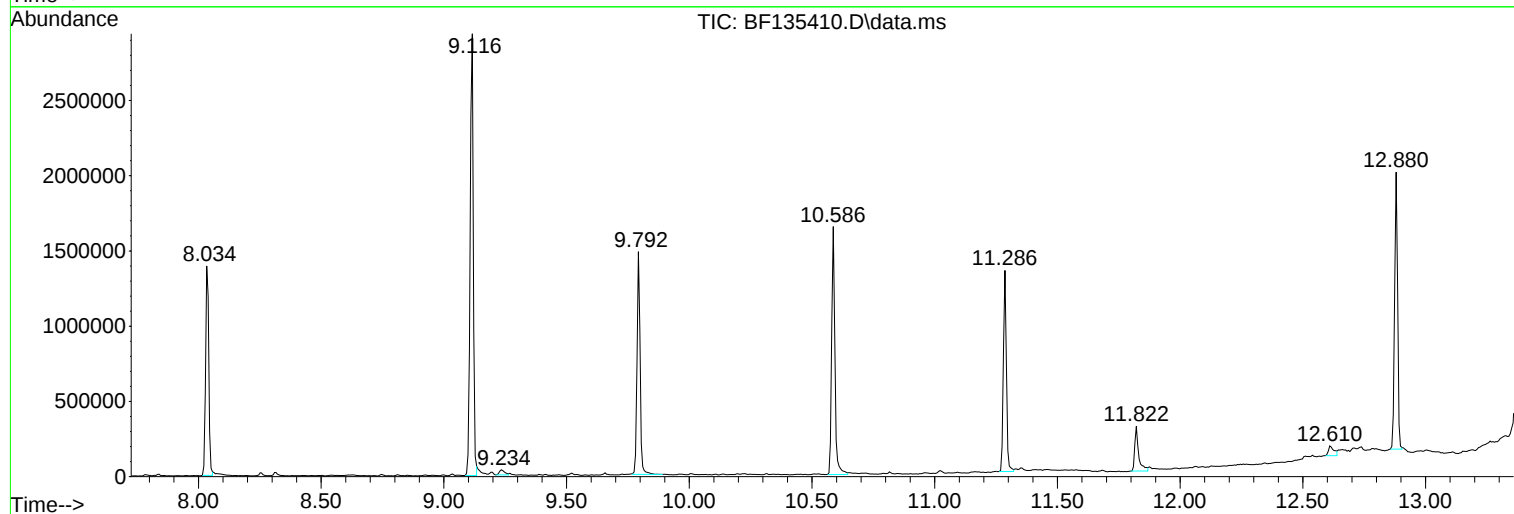
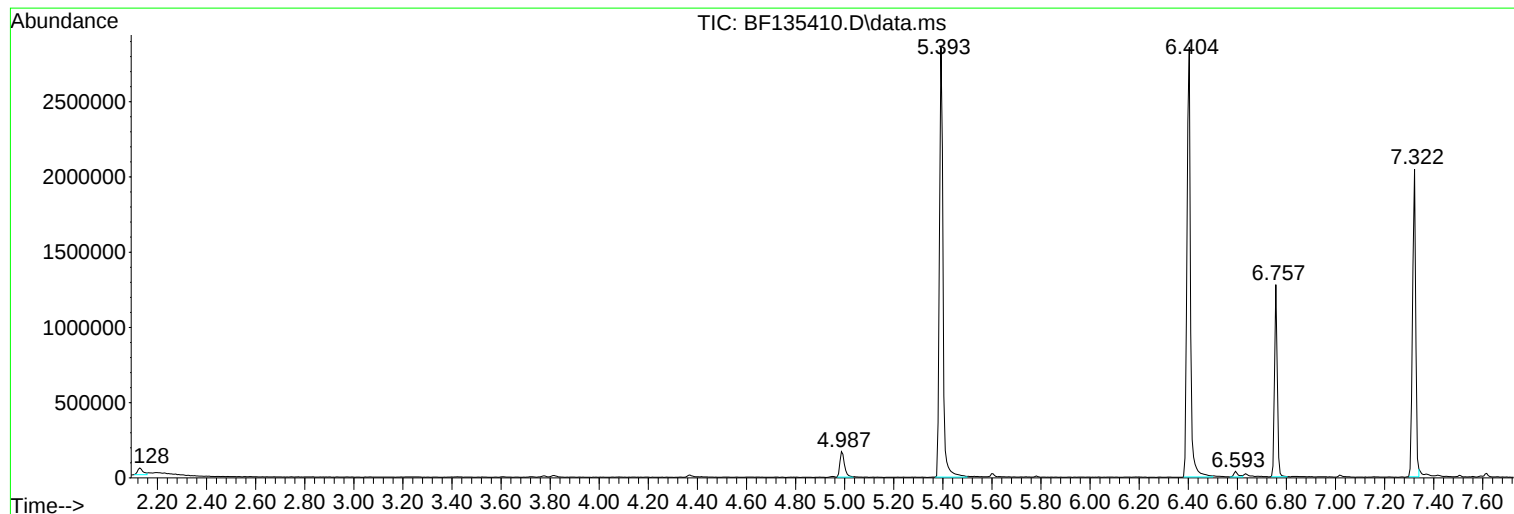
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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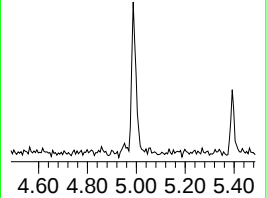
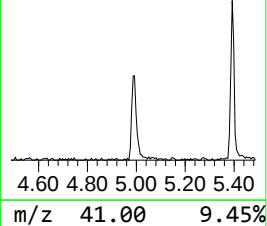
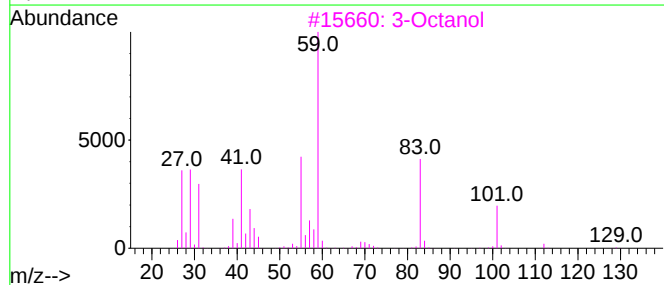
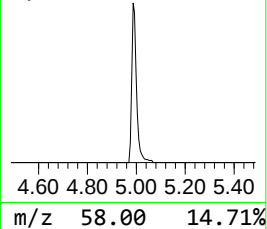
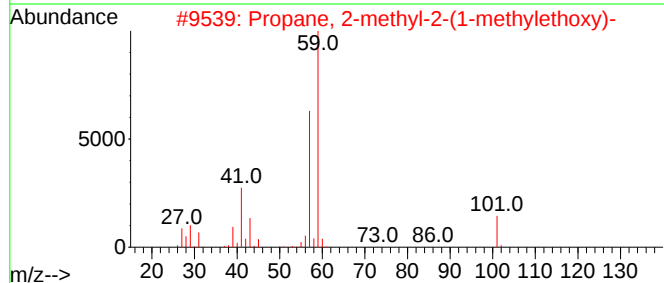
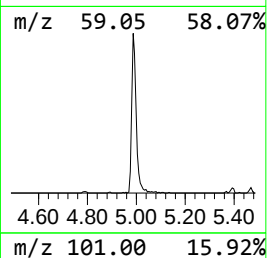
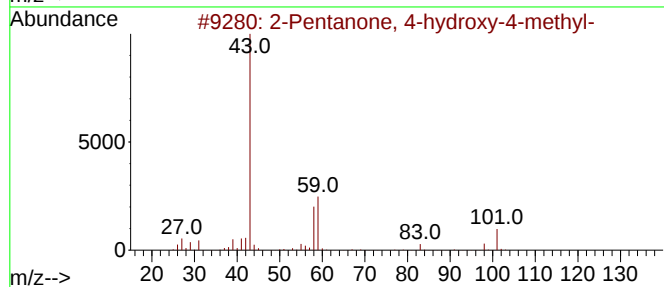
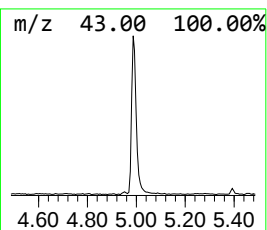
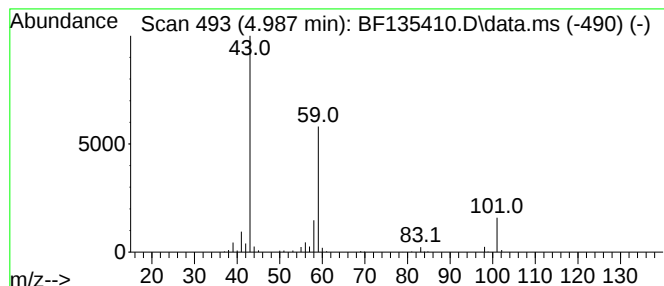
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.987	4.37 ng	218291	1,4-Dichlorobenzene-d4	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53		
3	3-Octanol	130	C8H18O	000589-98-0	33		
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		



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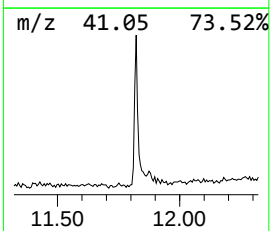
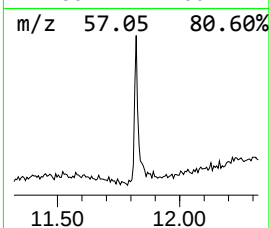
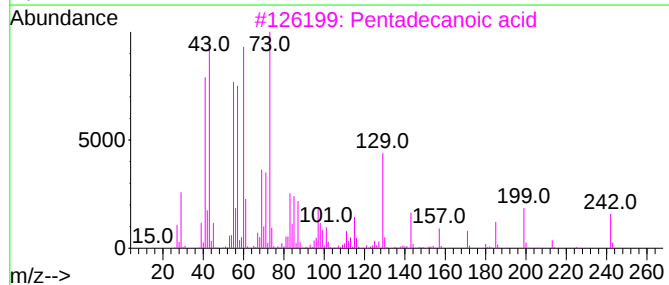
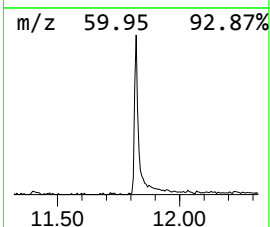
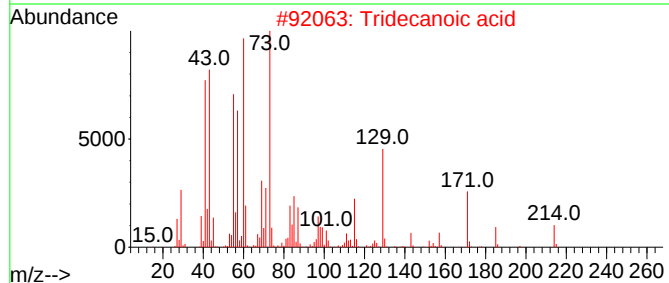
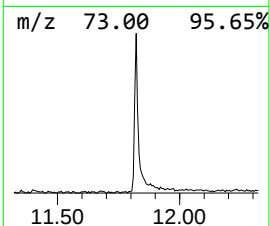
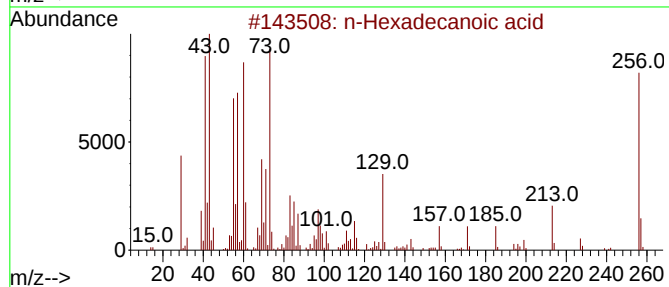
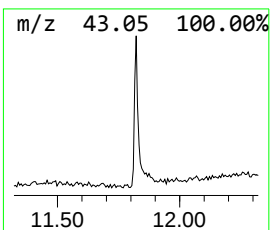
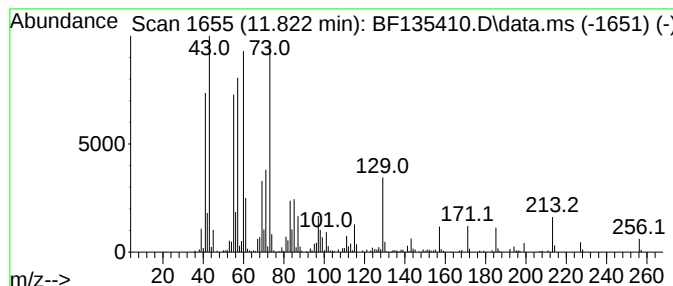
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.822	5.76 ng	332482	Phenanthrene-d10	11.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	92
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Undecanoic acid	186	C11H22O2	000112-37-8	81
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	80



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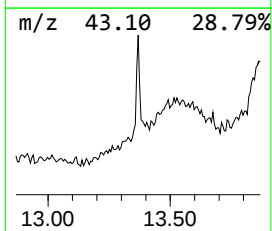
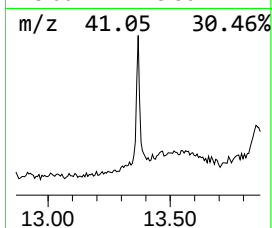
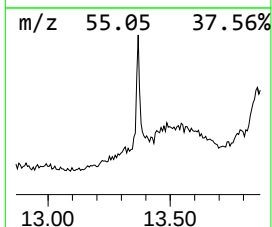
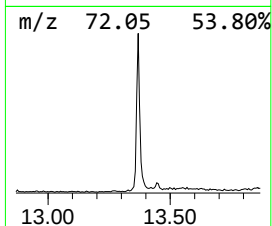
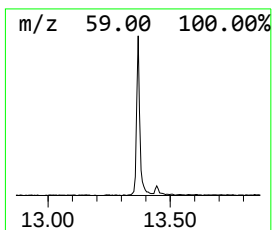
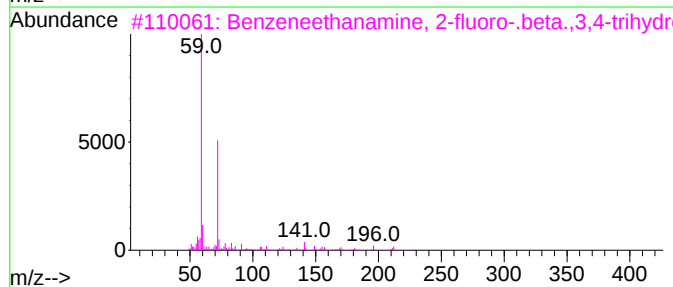
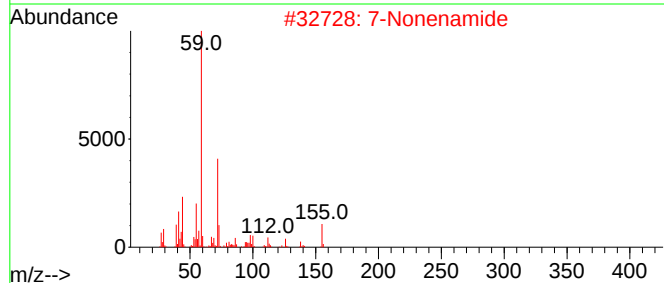
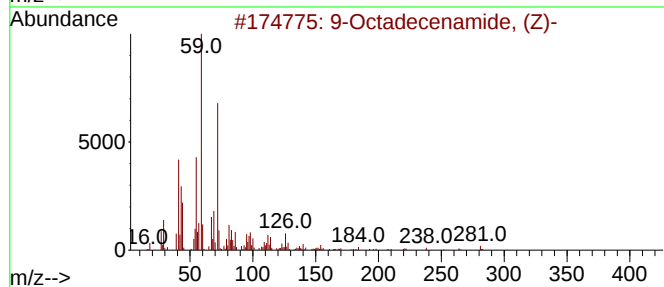
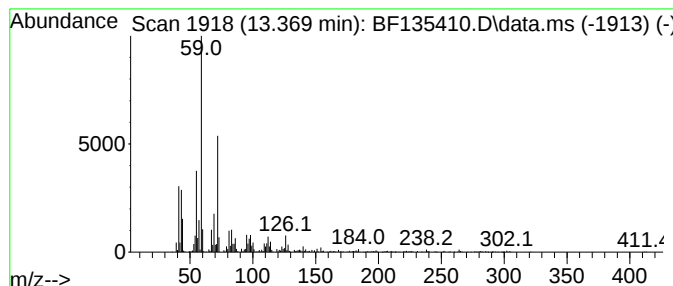
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Peak Number 3 9-Octadecenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.368	9.79 ng	520217	Chrysene-d12	13.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2			7-Nonenamide	155	C9H17NO	090949-53-4	72
3			Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	64
4			Dodecanamide	199	C12H25NO	001120-16-7	59
5			Nonanamide	157	C9H19NO	001120-07-6	59



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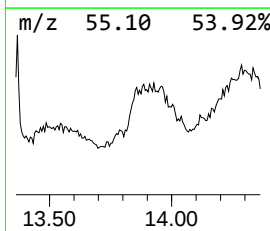
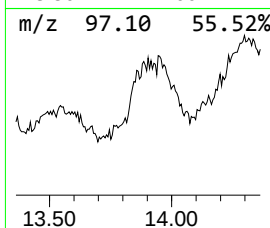
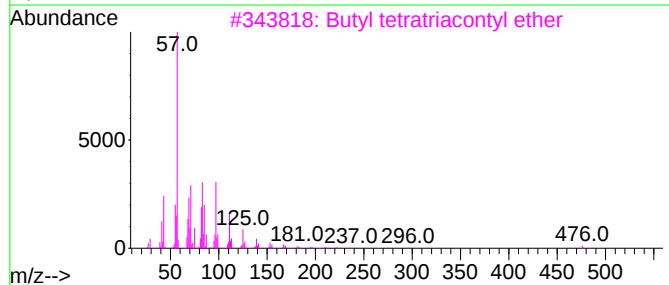
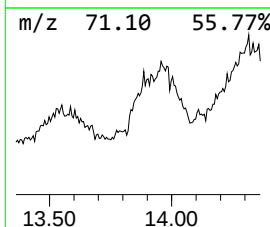
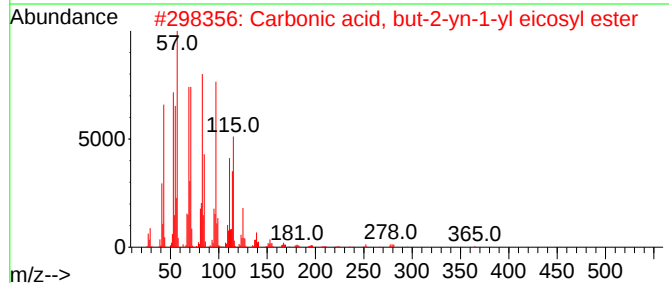
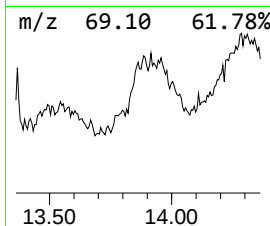
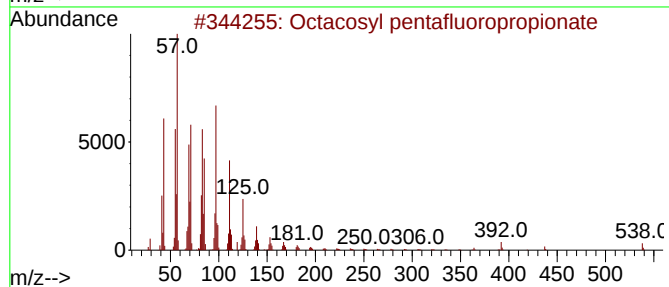
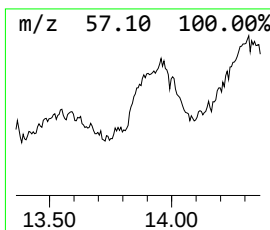
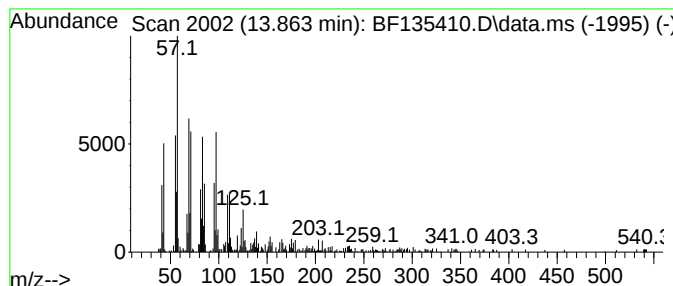
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Peak Number 4 Octacosyl pentafluoropropio... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.863	6.61 ng	351255	Chrysene-d12	13.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosyl pentafluoropropionate	556	C31H57F5O2	1000351-88-9	60
2			Carbonic acid, but-2-yn-1-yl eic...	394	C25H46O3	1000383-21-4	58
3			Butyl tetratriacontyl ether	551	C38H78O	1000406-41-4	58
4			Tetracosyl pentafluoropropionate	500	C27H49F5O2	1000351-81-3	53
5			Propyl tetratriacontyl ether	537	C37H76O	1000406-28-8	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.987	4.4	ng	218291	1	6.757	999592	20.0
n-Hexadecanoic ...	11.822	5.8	ng	332482	4	11.286	1154480	20.0
9-Octadecenamid...	13.368	9.8	ng	520217	5	13.945	1062770	20.0
Octacosyl penta...	13.863	6.6	ng	351255	5	13.945	1062770	20.0