

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100923\
 Data File : BF135646.D
 Acq On : 09 Oct 2023 11:58
 Operator : CG\JU
 Sample : 04778-10
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NBS-GROUNDWATER

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: BF135646.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	3	15	16	rBV2	20961	66608	1.72%	0.294%
2	4.957	485	488	498	rBV	161589	195777	5.06%	0.863%
3	5.375	556	559	575	rBV	1526898	1774271	45.81%	7.819%
4	6.387	728	731	747	rBV	1052069	1148429	29.65%	5.061%
5	6.740	787	791	799	rBV	887769	787730	20.34%	3.471%
6	7.304	883	887	897	rBV	2230748	2417796	62.43%	10.654%
7	8.016	1004	1008	1014	rBV	1189157	1036297	26.76%	4.567%
8	9.098	1186	1192	1195	rBV	4194866	3872883	100.00%	17.066%
9	9.216	1208	1212	1224	rVB	359833	357933	9.24%	1.577%
10	9.775	1303	1307	1310	rBV	1350650	1133063	29.26%	4.993%
11	9.810	1310	1313	1316	rVB	426586	382882	9.89%	1.687%
12	10.328	1398	1401	1404	rBV	57406	49066	1.27%	0.216%
13	10.486	1426	1428	1434	rBV6	27272	49252	1.27%	0.217%
14	10.575	1439	1443	1455	rVV	2414132	2458705	63.49%	10.835%
15	11.269	1558	1561	1564	rBV	1251367	1129488	29.16%	4.977%
16	11.810	1650	1653	1663	rVB	575345	600579	15.51%	2.647%
17	12.375	1747	1749	1753	rVB2	66700	56394	1.46%	0.249%
18	12.498	1767	1770	1772	rBV	67922	71152	1.84%	0.314%
19	12.598	1784	1787	1796	rVB	417647	452590	11.69%	1.994%
20	12.869	1829	1833	1837	rBV	3036729	3121453	80.60%	13.755%
21	13.933	2011	2014	2021	rVB	745158	679576	17.55%	2.995%
22	14.774	2153	2157	2163	rVB	107100	113573	2.93%	0.500%
23	15.404	2259	2264	2270	rBV	591286	737506	19.04%	3.250%

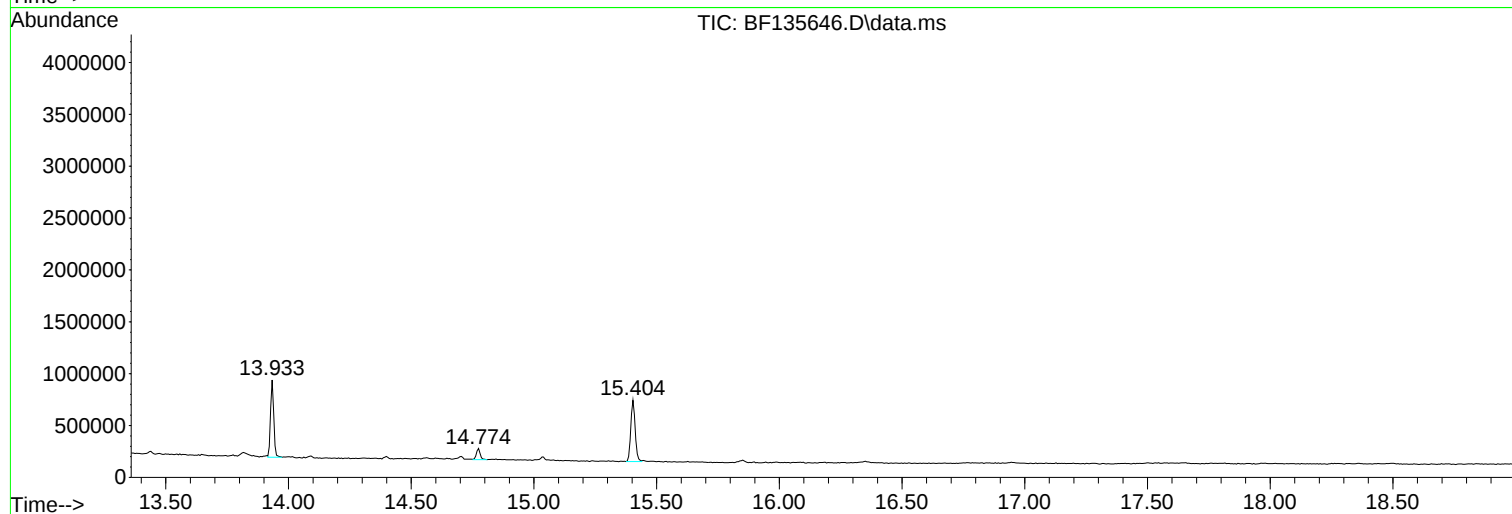
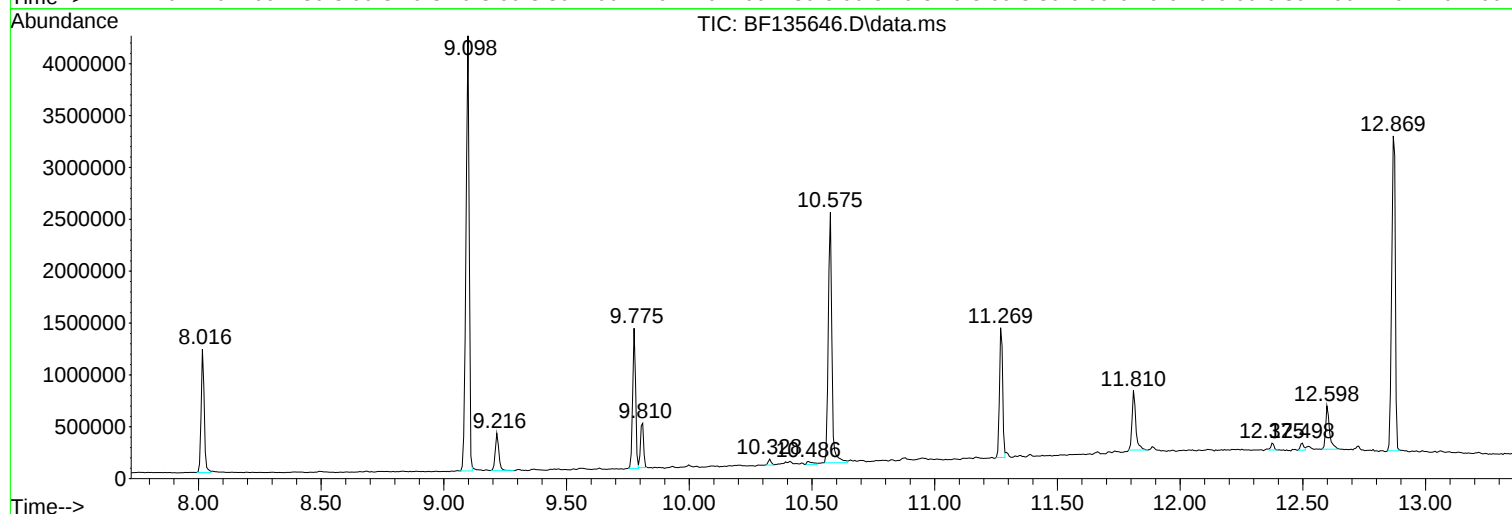
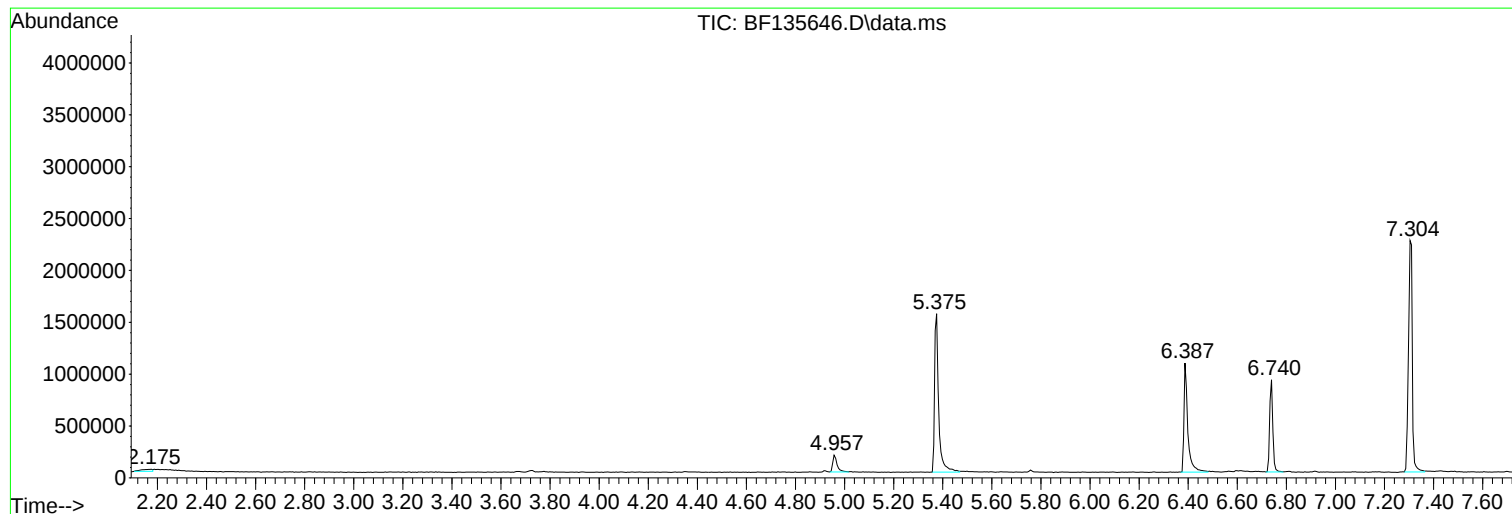
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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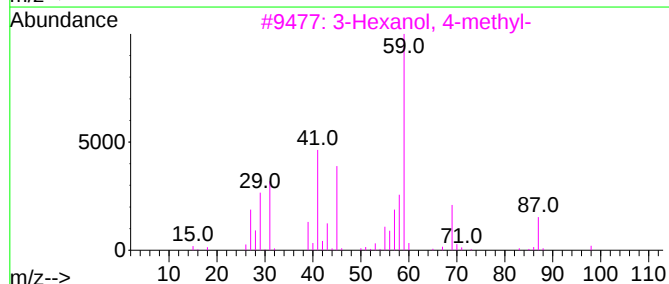
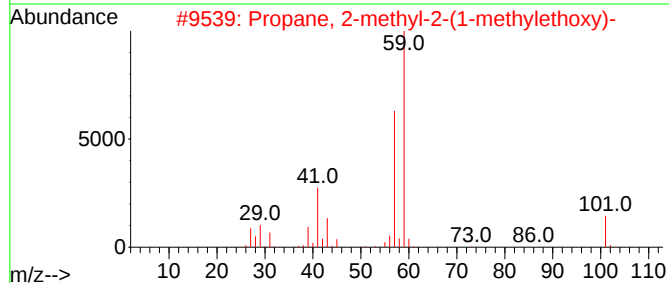
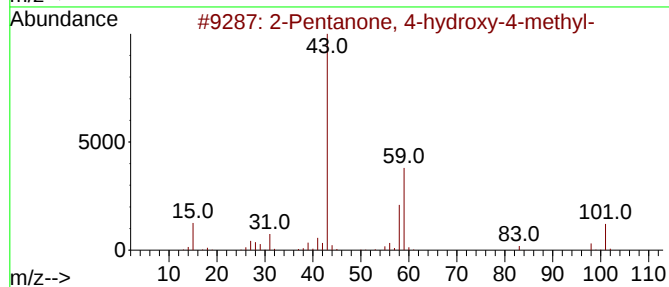
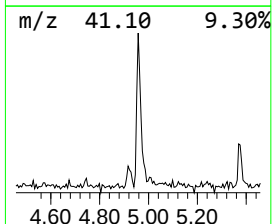
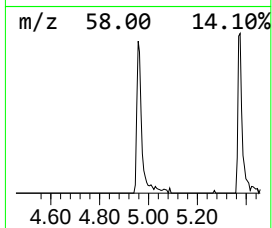
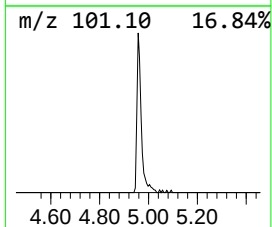
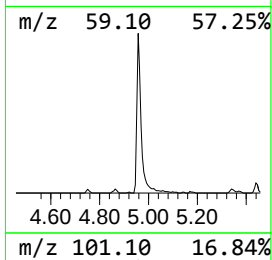
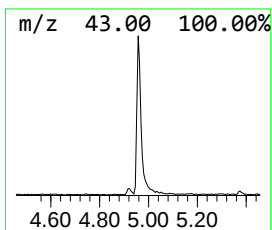
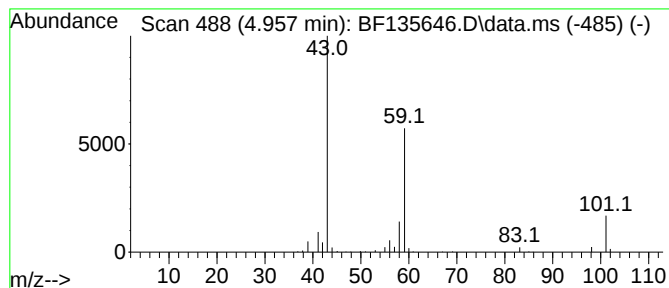
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.957	4.97 ng	195777	1,4-Dichlorobenzene-d4	6.740

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36		
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		



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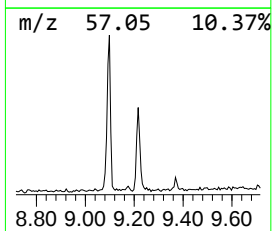
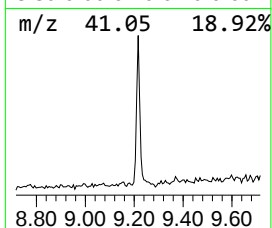
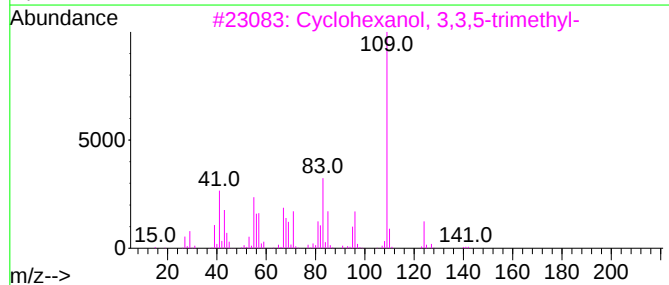
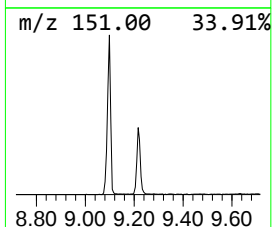
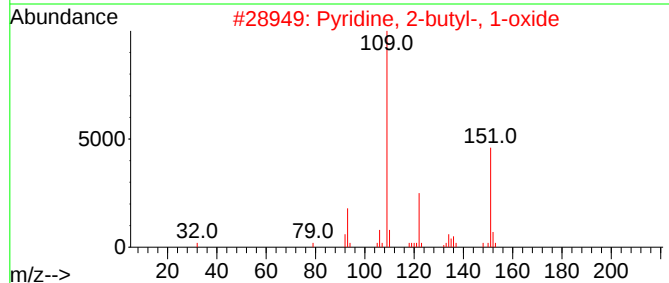
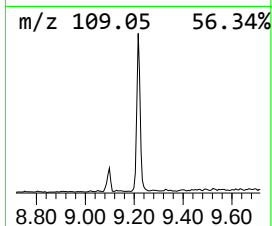
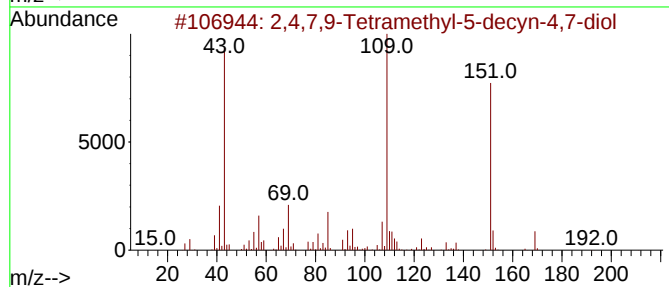
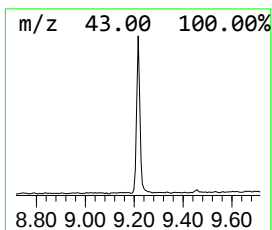
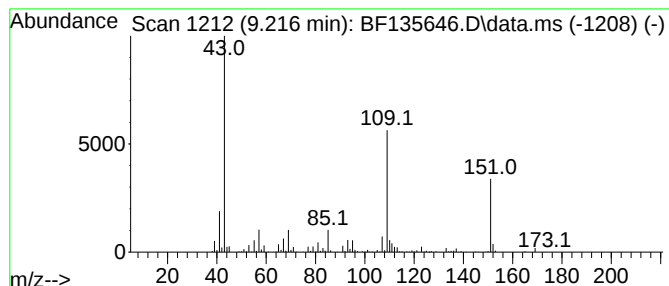
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Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.216	6.32 ng	357933	Acenaphthene-d10	9.775

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	87	
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	53	
3	Cyclohexanol, 3,3,5-trimethyl-	142	C9H18O	000116-02-9	50	
4	Metacetamol	151	C8H9NO2	000621-42-1	47	
5	2-Thiophenecarbonitrile	109	C5H3NS	001003-31-2	47	



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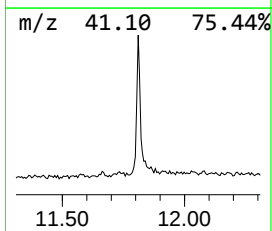
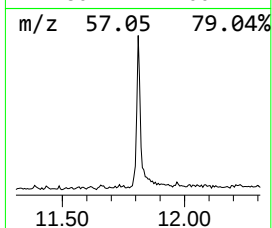
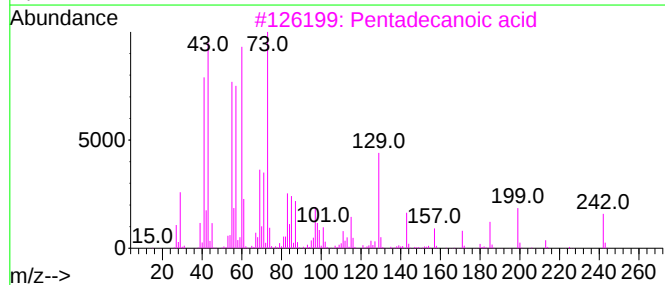
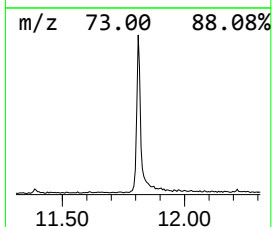
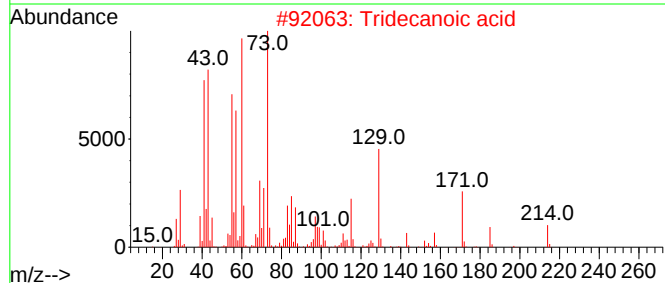
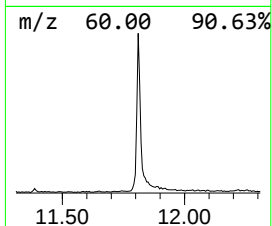
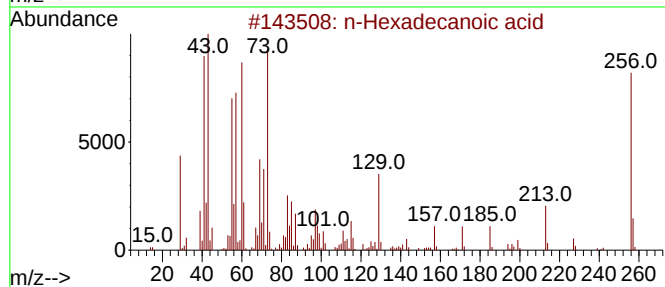
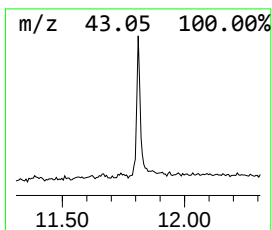
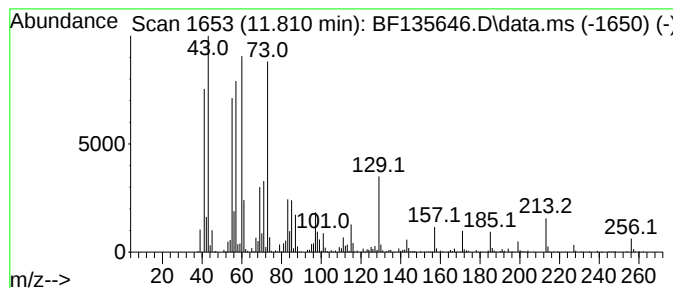
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.810	10.63 ng	600579	Phenanthrene-d10	11.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			Dodecanoic acid	200	C12H24O2	000143-07-7	68



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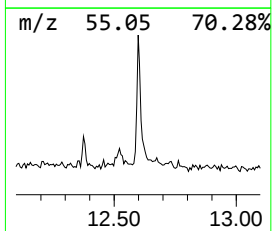
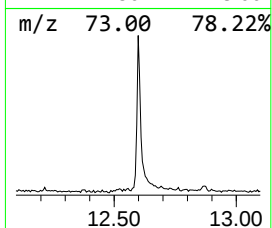
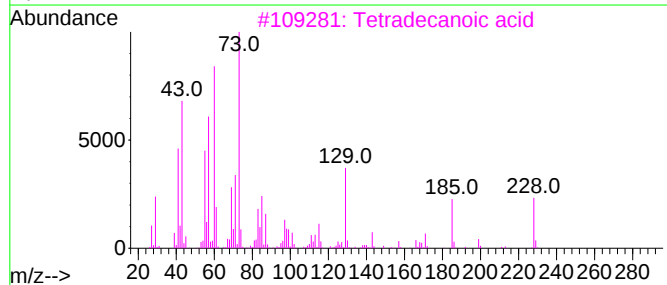
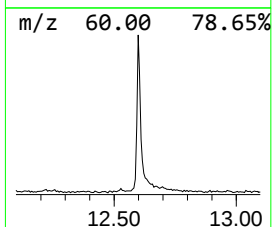
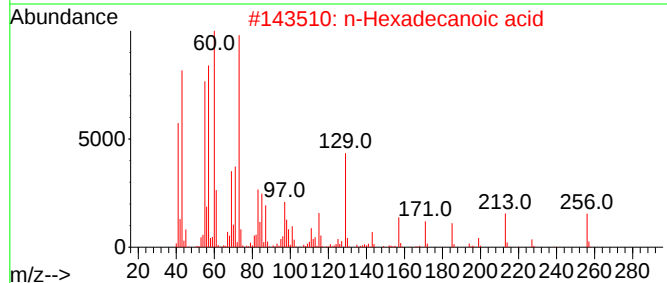
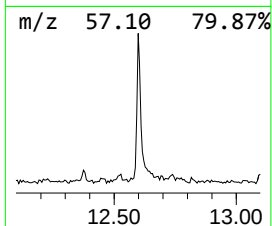
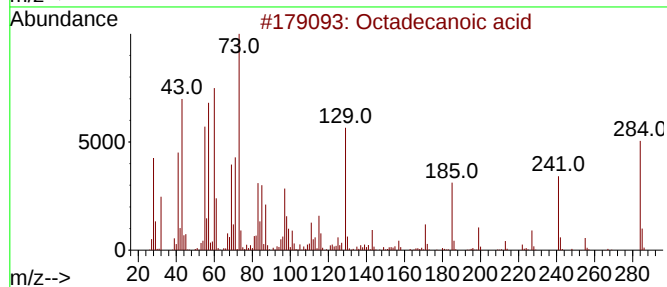
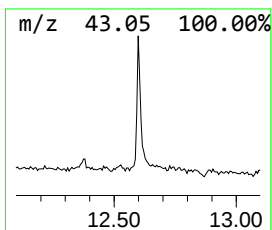
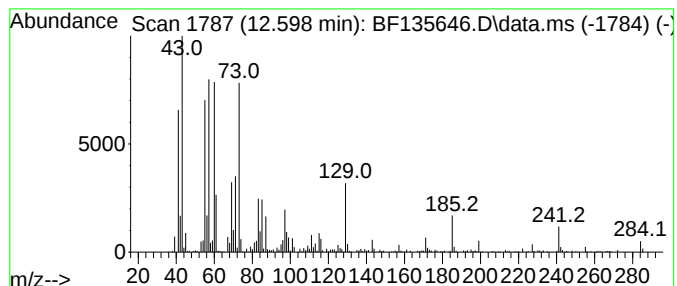
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Peak Number 4 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.598	8.01 ng	452590	Phenanthrene-d10	11.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	97
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4			Tridecanoic acid	214	C13H26O2	000638-53-9	64
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64



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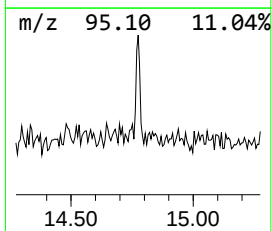
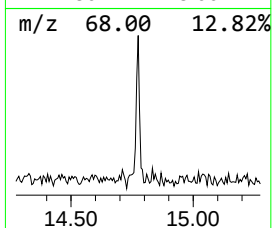
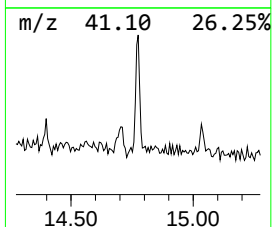
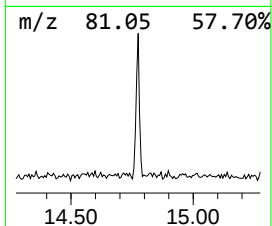
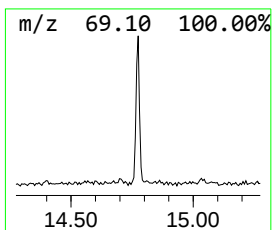
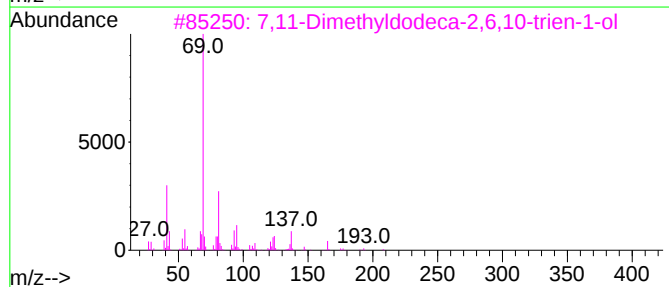
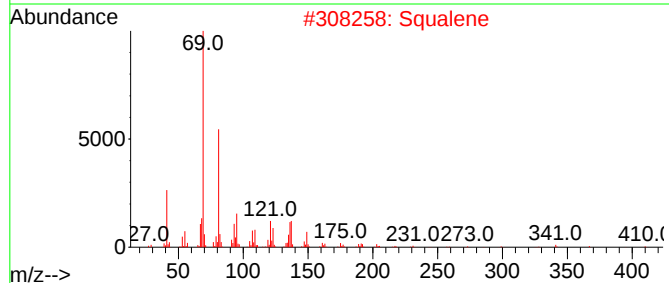
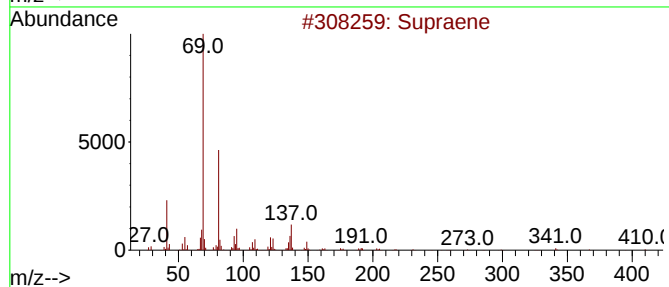
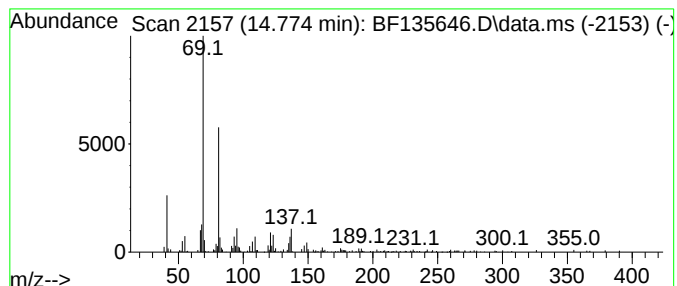
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Peak Number 5 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.774	3.08 ng	113573	Perylene-d12	15.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			Squalene	410	C30H50	000111-02-4	90
3			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
4			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
5			Ethyl 5,9,13-trimethyl-(2E,4E,8Z...	290	C19H30O2	1000432-28-7	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.957	5.0	ng	195777	1	6.740	787730	20.0
2,4,7,9-Tetrame...	9.216	6.3	ng	357933	3	9.775	1133060	20.0
n-Hexadecanoic ...	11.810	10.6	ng	600579	4	11.269	1129490	20.0
Octadecanoic acid	12.598	8.0	ng	452590	4	11.269	1129490	20.0
Supraene	14.774	3.1	ng	113573	6	15.404	737506	20.0