

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100324\
 Data File : BF139640.D
 Acq On : 03 Oct 2024 19:22
 Operator : RC/JU
 Sample : P4236-05
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP3

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-BF100124.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139640.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.157	3	11	26	rVB	1548022	2441986	100.00%	14.830%
2	5.081	498	508	515	rVB	90149	139096	5.70%	0.845%
3	5.487	571	577	582	rBV	1317541	1719327	70.41%	10.441%
4	6.492	742	748	753	rBV	1338371	1768718	72.43%	10.741%
5	6.863	806	811	816	rBV	401588	486165	19.91%	2.952%
6	7.428	901	907	912	rBV	857706	1155158	47.30%	7.015%
7	8.145	1024	1029	1034	rBV	507821	623107	25.52%	3.784%
8	9.222	1206	1212	1217	rBV	1603754	2061968	84.44%	12.522%
9	9.898	1322	1327	1332	rBV	564413	693921	28.42%	4.214%
10	10.610	1443	1448	1454	rVB	54389	66986	2.74%	0.407%
11	10.686	1456	1461	1477	rBV	935487	1200371	49.16%	7.290%
12	11.386	1574	1580	1588	rBV	565512	722177	29.57%	4.386%
13	11.910	1659	1669	1681	rBV2	142273	227869	9.33%	1.384%
14	12.598	1780	1786	1794	rBV	31432	40380	1.65%	0.245%
15	12.692	1797	1802	1811	rBV	19238	34686	1.42%	0.211%
16	12.827	1816	1825	1831	rVB	28709	43535	1.78%	0.264%
17	12.968	1844	1849	1854	rBV	1455633	1858724	76.12%	11.288%
18	13.880	1998	2004	2019	rBV2	47294	119332	4.89%	0.725%
19	14.021	2020	2028	2038	rVB	384746	541630	22.18%	3.289%
20	15.062	2201	2205	2213	rVB	12789	27669	1.13%	0.168%
21	15.492	2272	2278	2289	rVB	319848	493655	20.22%	2.998%

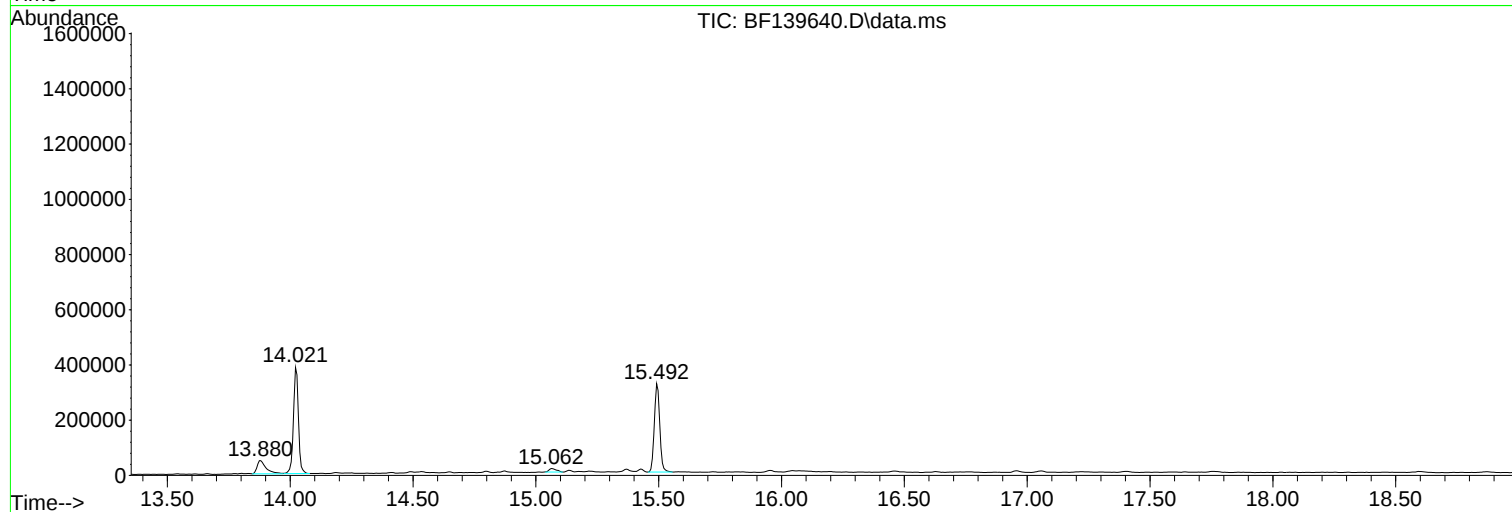
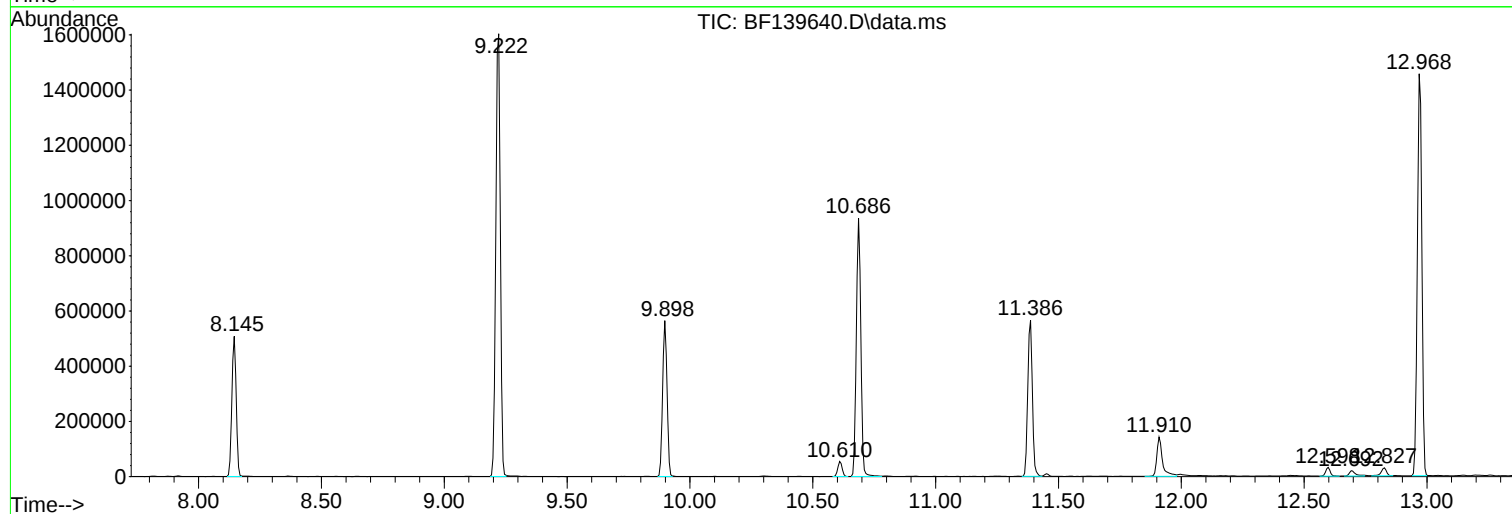
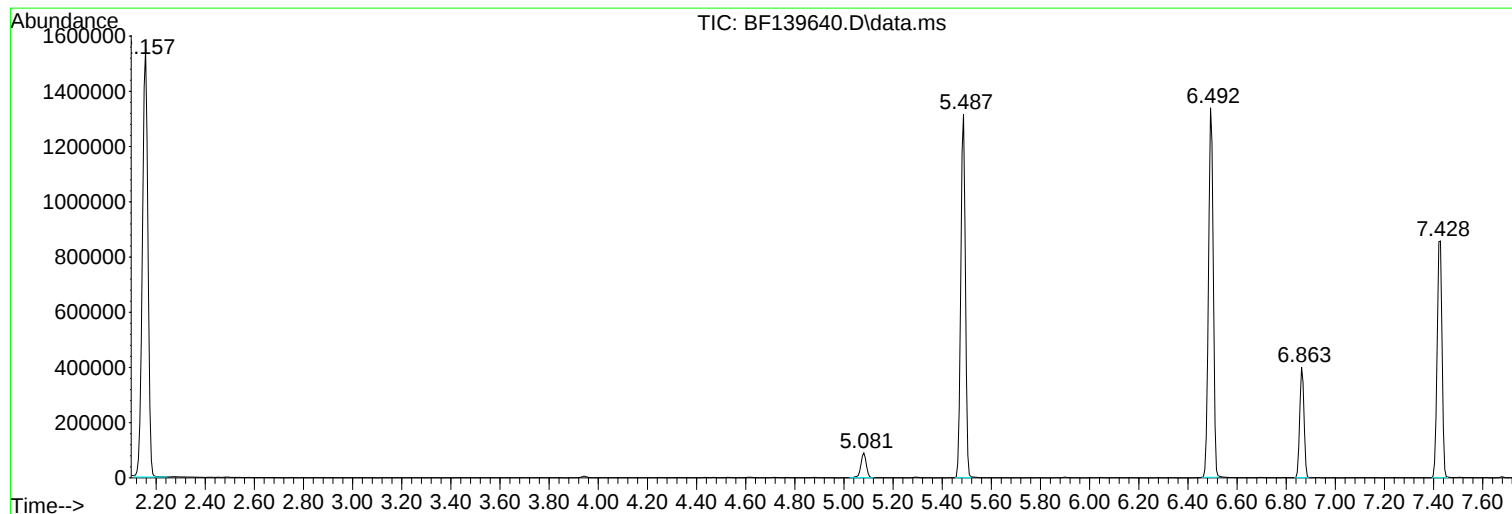
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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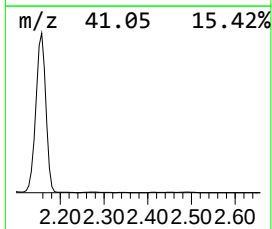
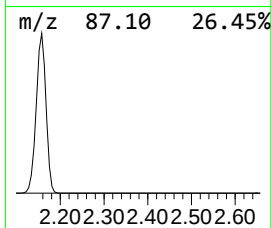
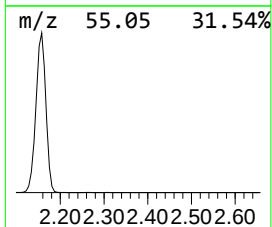
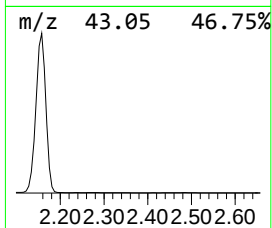
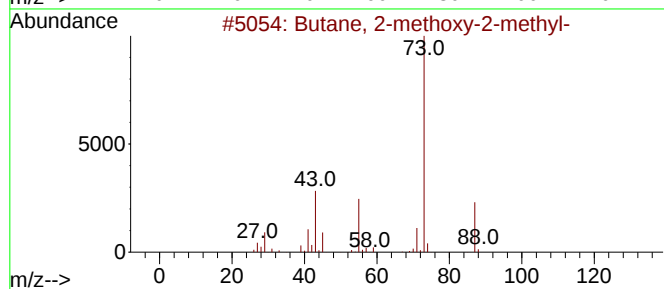
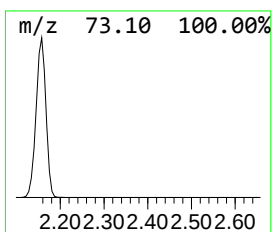
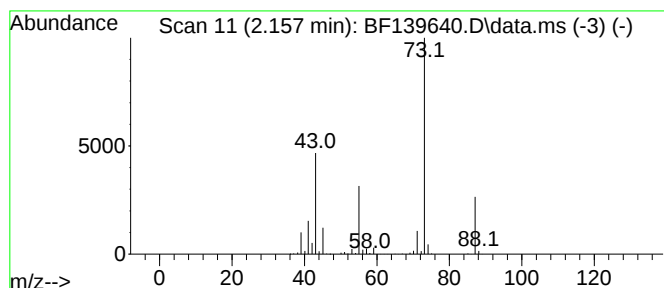
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.157	100.46 ng	2441990	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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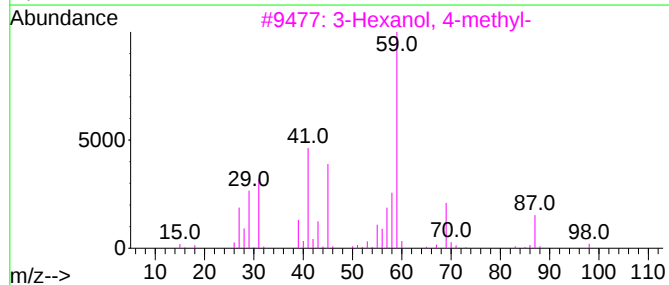
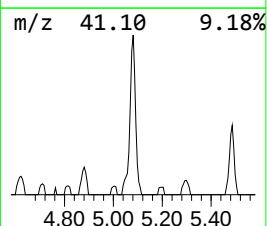
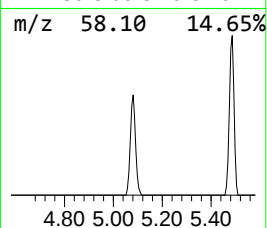
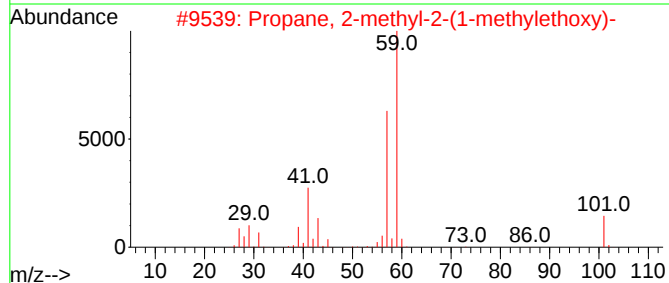
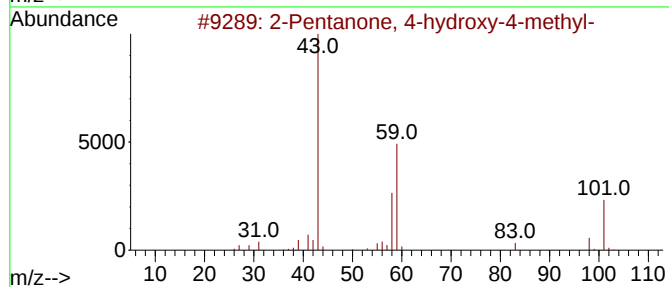
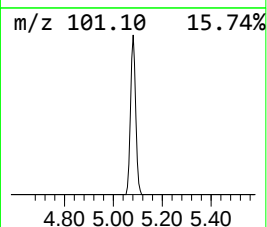
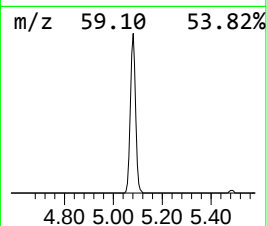
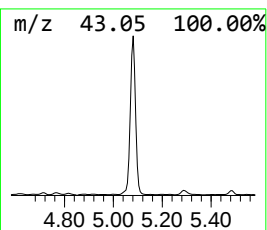
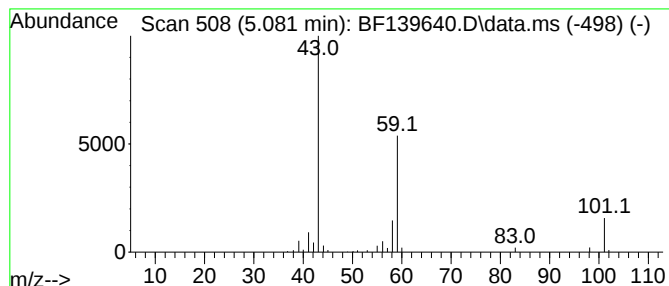
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.081	5.72 ng	139096	1,4-Dichlorobenzene-d4	6.863

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	33
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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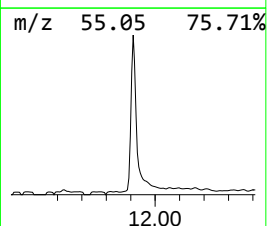
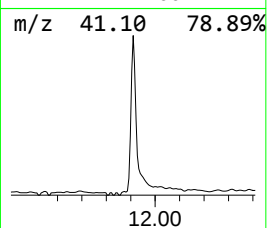
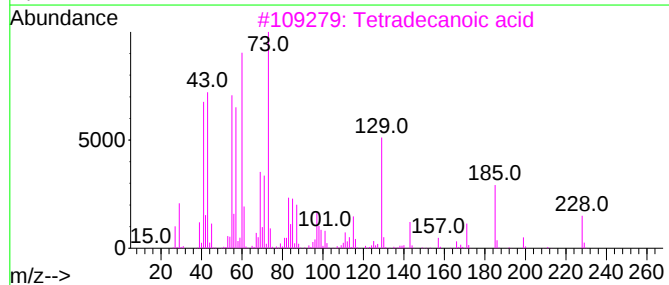
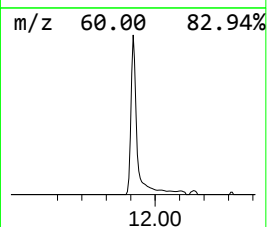
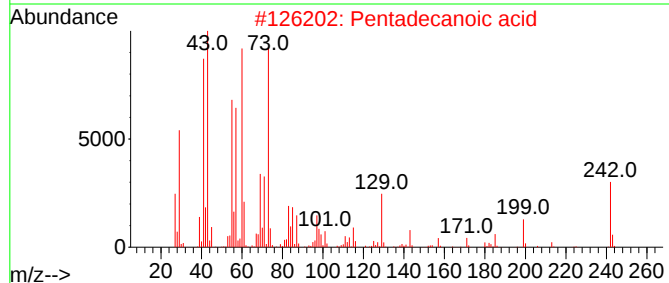
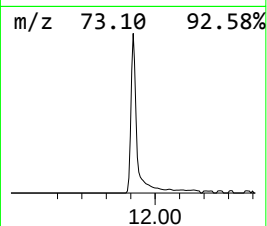
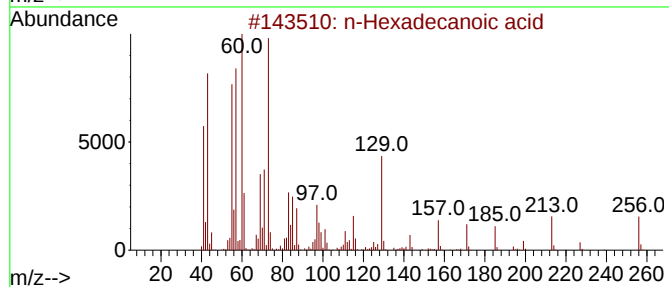
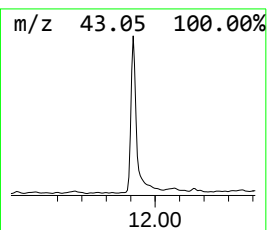
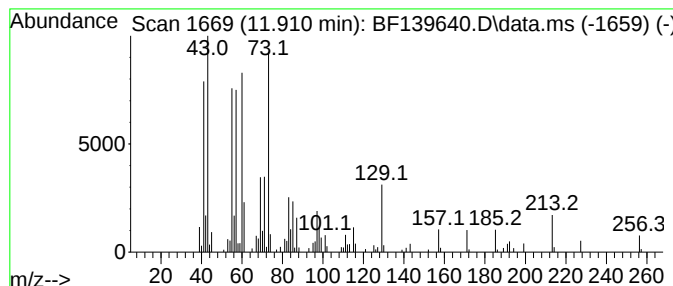
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.910	6.31 ng	227869	Phenanthrene-d10	11.386

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4		Tridecanoic acid	214	C13H26O2	000638-53-9	68
5		Trehalose	342	C12H22O11	000099-20-7	50



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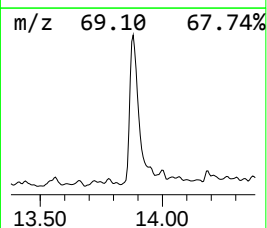
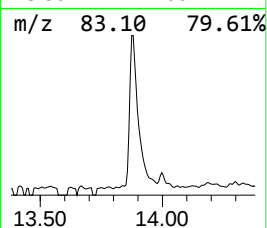
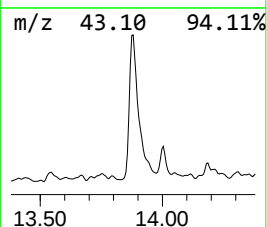
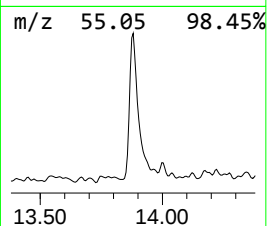
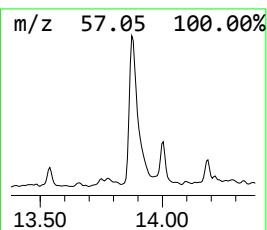
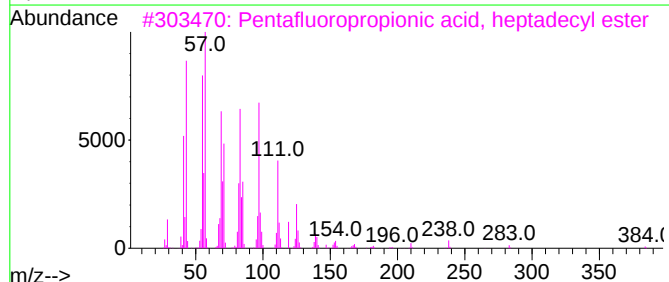
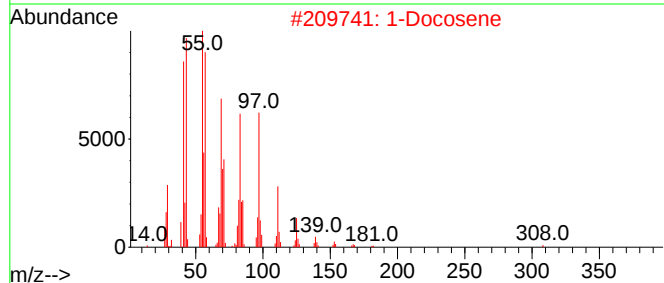
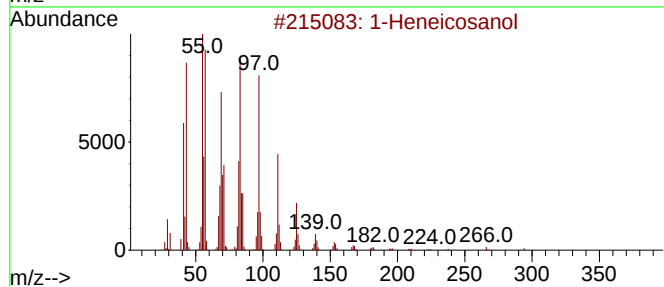
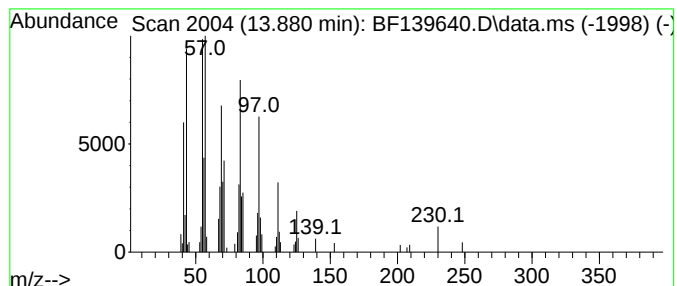
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Peak Number 4 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	4.41 ng	119332	Chrysene-d12	14.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	95
2			1-Docosene	308	C22H44	001599-67-3	94
3			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
4			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
5			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.157	100.5	ng	2441990	1	6.863	486165	20.0
2-Pentanone, 4-...	5.081	5.7	ng	139096	1	6.863	486165	20.0
n-Hexadecanoic ...	11.910	6.3	ng	227869	4	11.386	722177	20.0
1-Heneicosanol	13.880	4.4	ng	119332	5	14.021	541630	20.0