

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020723\
 Data File : BG056569.D
 Acq On : 7 Feb 2023 15:59
 Operator : CG/JU
 Sample : 01463-05
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 COMP-5

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_G\Methods\8270-BG012723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056569.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.300	336	342	349	rBV	97965	153097	6.89%	1.539%
2	5.794	418	426	439	rBV	402591	652828	29.40%	6.564%
3	7.416	694	702	716	rBV	396293	699356	31.50%	7.032%
4	8.268	840	847	855	rBB	112332	183689	8.27%	1.847%
5	9.443	1039	1047	1058	rBB	233989	424069	19.10%	4.264%
6	11.100	1322	1329	1338	rBV	148368	264055	11.89%	2.655%
7	13.514	1732	1740	1747	rBV	961891	1420715	63.98%	14.286%
8	14.889	1967	1974	1981	rVB	285428	437114	19.69%	4.395%
9	16.229	2194	2202	2207	rVB	20774	30895	1.39%	0.311%
10	16.370	2220	2226	2238	rBV	683758	1026237	46.22%	10.319%
11	17.627	2433	2440	2445	rBV	378891	565968	25.49%	5.691%
12	17.668	2445	2447	2452	rVB	30049	37299	1.68%	0.375%
13	18.473	2577	2584	2593	rBV3	48683	88029	3.96%	0.885%
14	18.697	2614	2622	2626	rBV2	13465	30826	1.39%	0.310%
15	19.660	2781	2786	2791	rBV	80458	114215	5.14%	1.148%
16	20.024	2844	2848	2854	rVB	85399	117392	5.29%	1.180%
17	20.207	2873	2879	2884	rBV	1702269	2220485	100.00%	22.328%
18	21.493	3093	3098	3108	rVB4	64603	127614	5.75%	1.283%
19	21.916	3162	3170	3176	rBV	360202	682258	30.73%	6.860%
20	23.626	3458	3461	3468	rVB	40995	78123	3.52%	0.786%
21	25.336	3744	3752	3763	rVB2	207234	590708	26.60%	5.940%

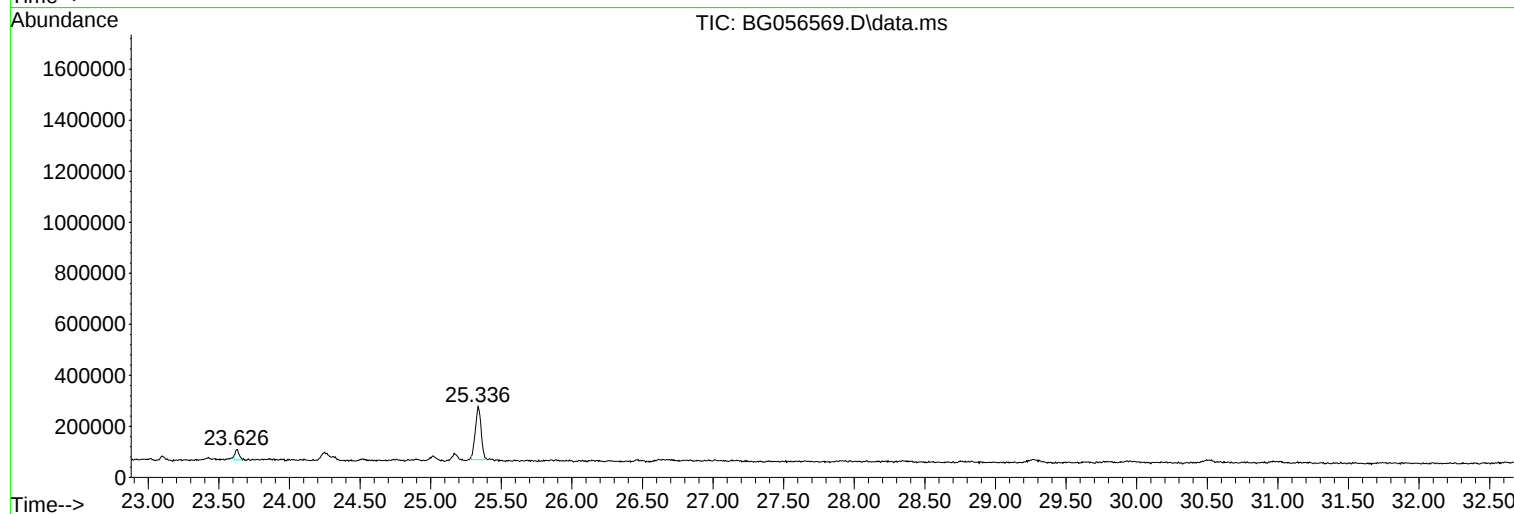
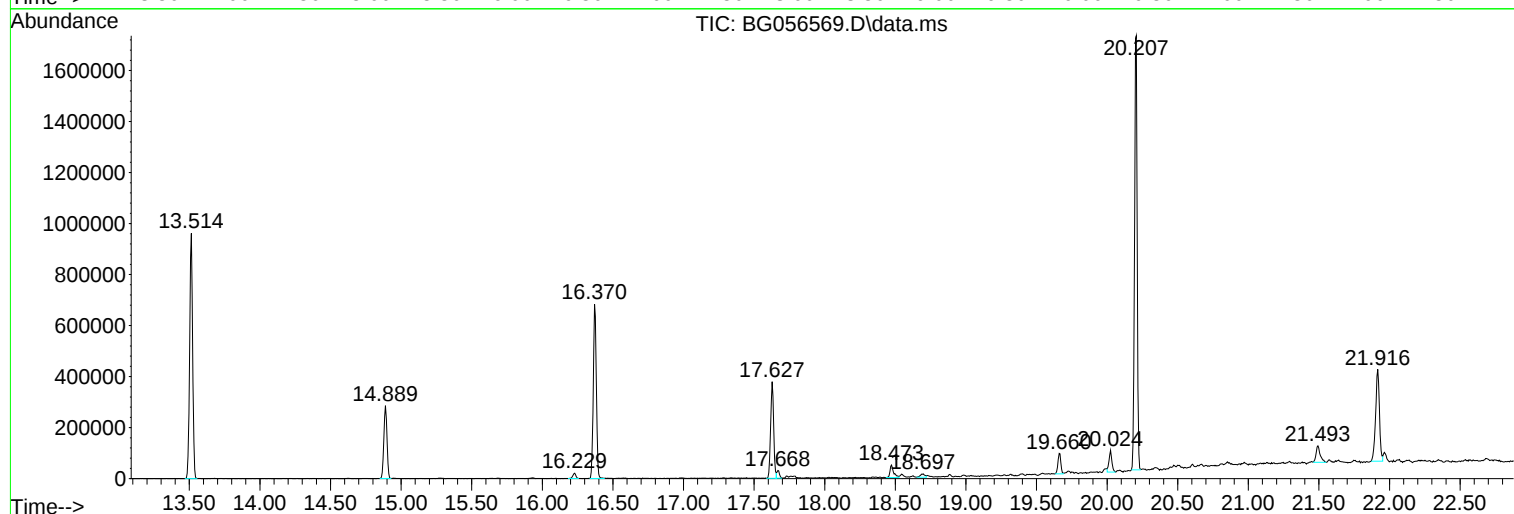
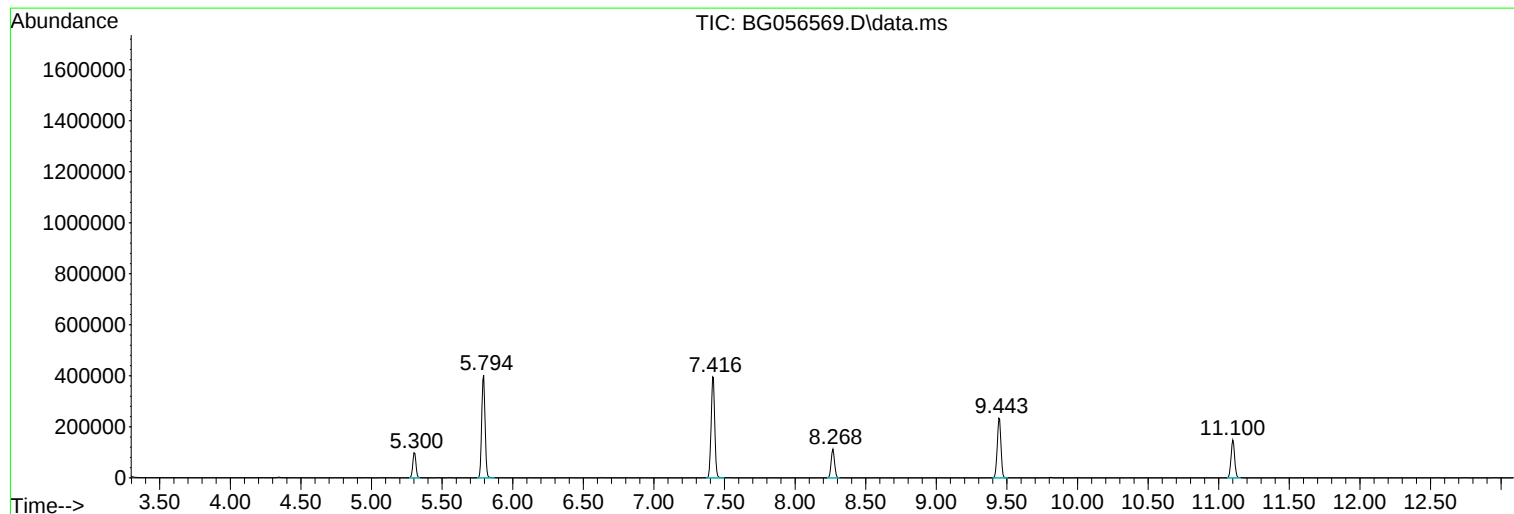
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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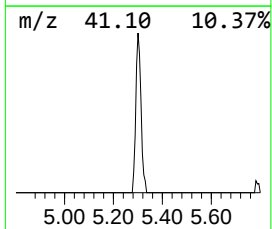
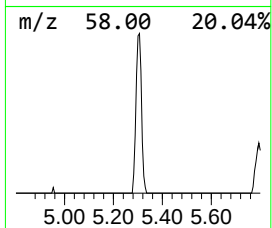
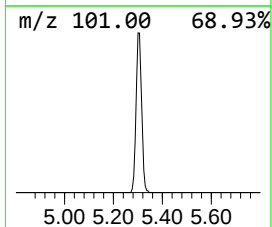
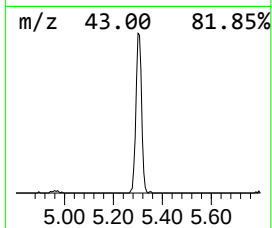
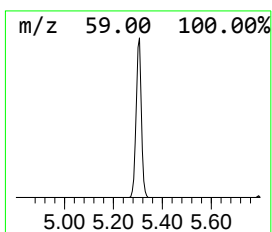
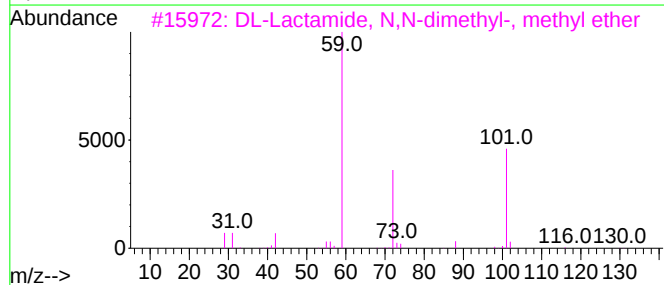
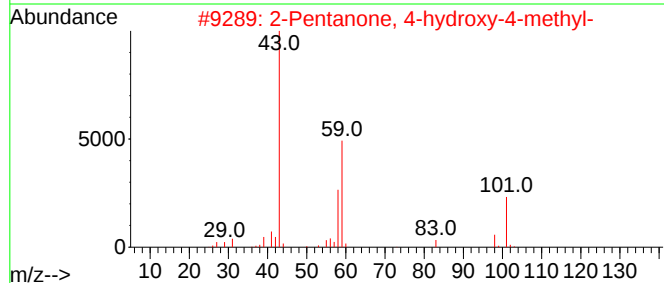
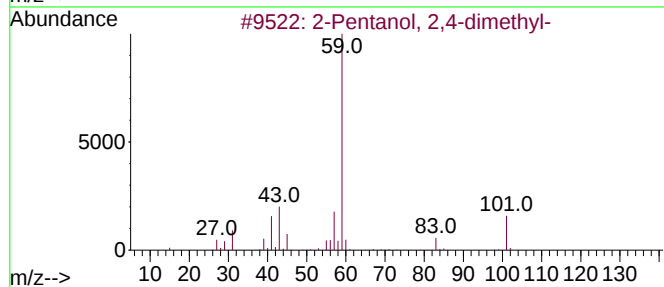
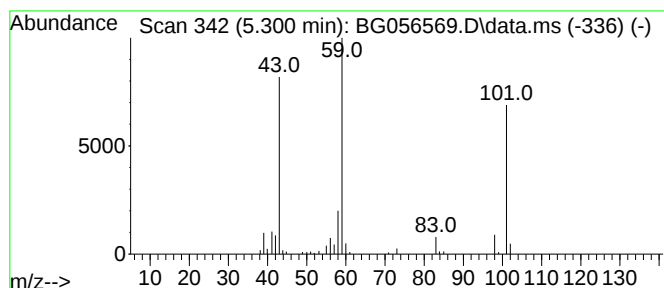
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanol, 2,4-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.300	16.67 ng	153097	1,4-Dichlorobenzene-d4	8.268

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	59
2			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
3			DL-Lactamide, N,N-dimethyl-, met...	131	C6H13NO2	1000452-57-0	40
4			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	35
5			Butanoic acid, 4-(2-methoxy-1-me...	204	C9H16O5	054966-46-0	33



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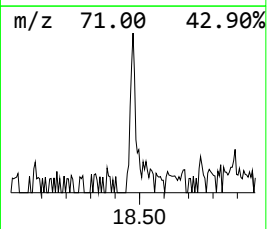
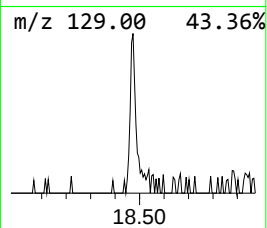
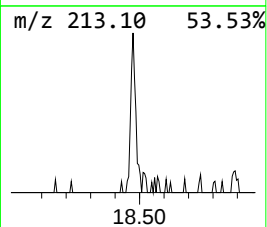
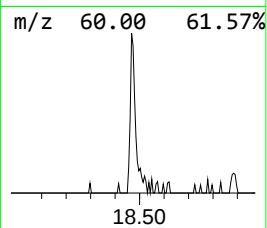
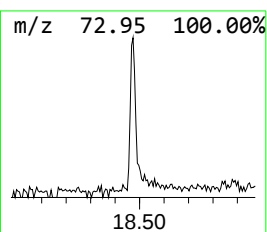
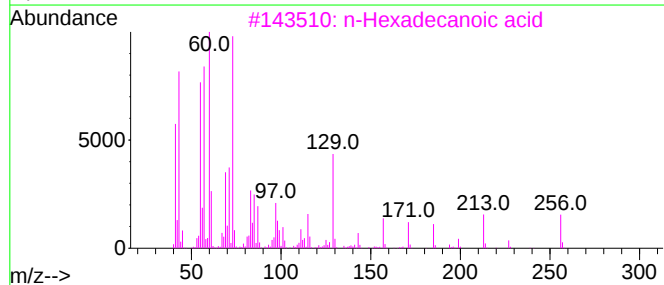
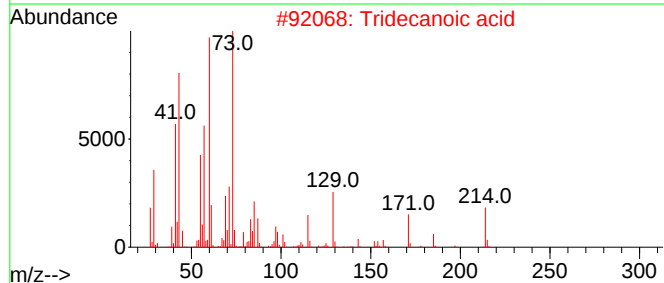
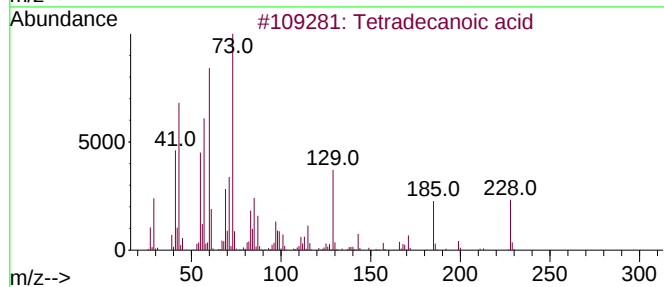
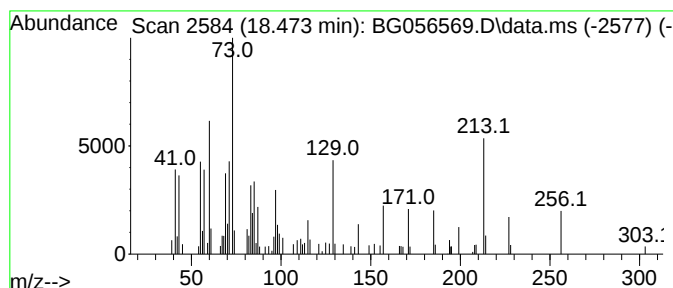
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Peak Number 2 Tetradecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.473	3.11 ng	88029	Phenanthrene-d10	17.627

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
2			Tridecanoic acid	214	C13H26O2	000638-53-9	60
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	60
4			n-Decanoic acid	172	C10H20O2	000334-48-5	42
5			Octadecanoic acid	284	C18H36O2	000057-11-4	35



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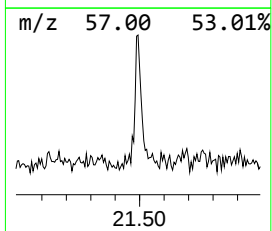
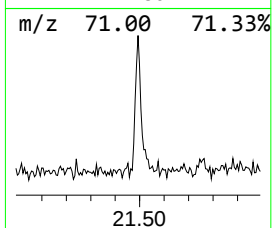
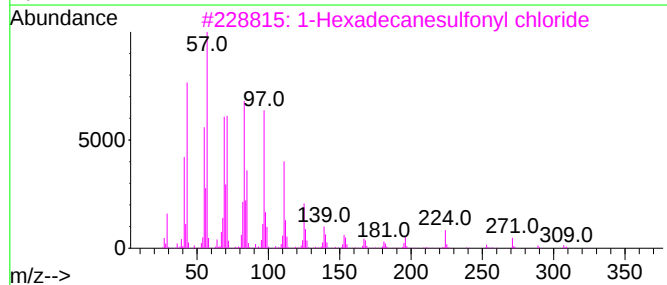
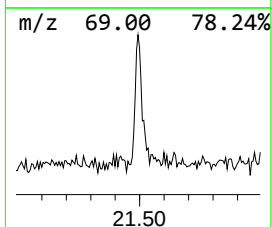
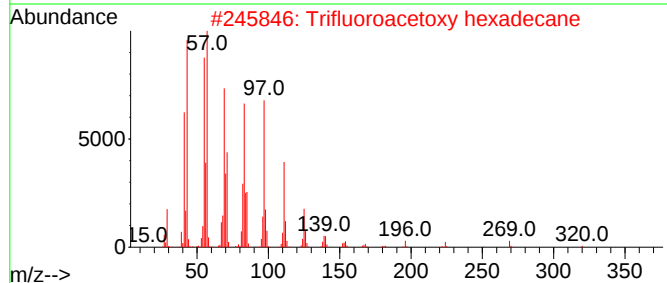
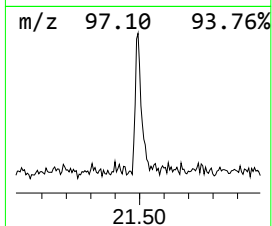
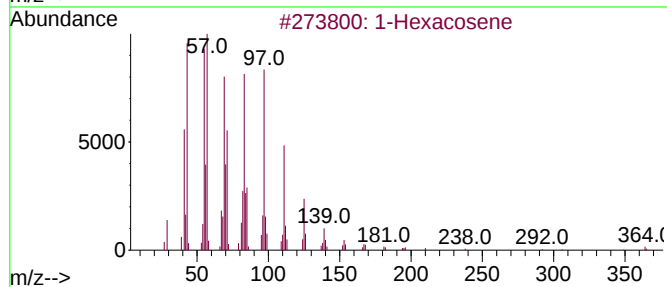
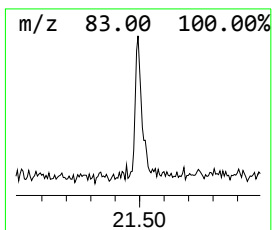
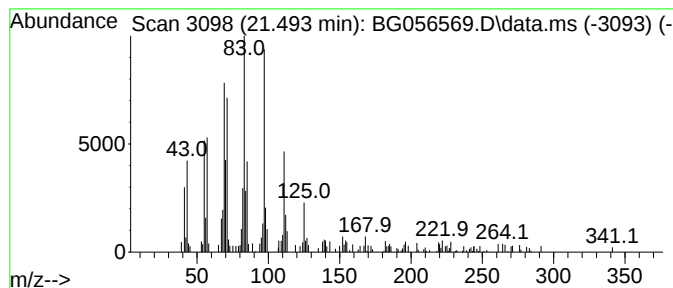
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Peak Number 3 1-Hexacosene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.493	3.74 ng	127614	Chrysene-d12	21.916	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene	364	C26H52	018835-33-1	90
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	83
3	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	81
4	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	81
5	1-Tricosene	322	C23H46	018835-32-0	81



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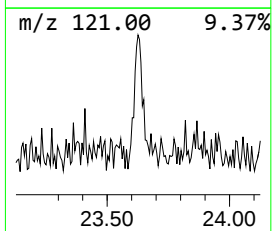
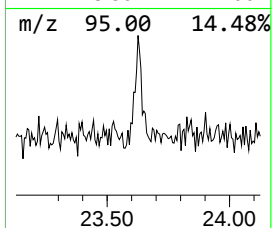
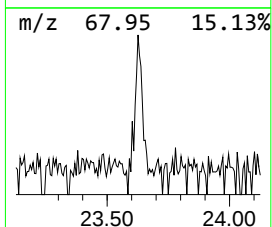
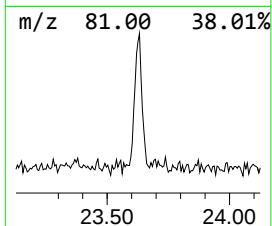
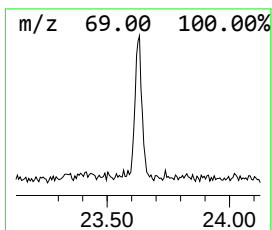
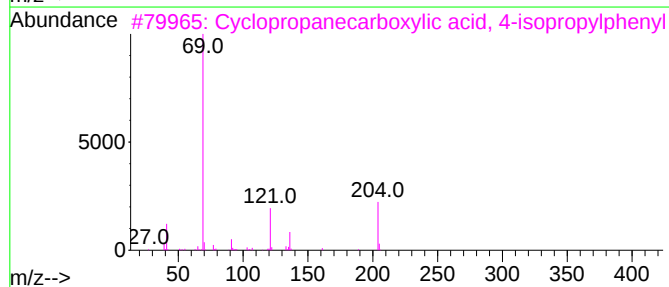
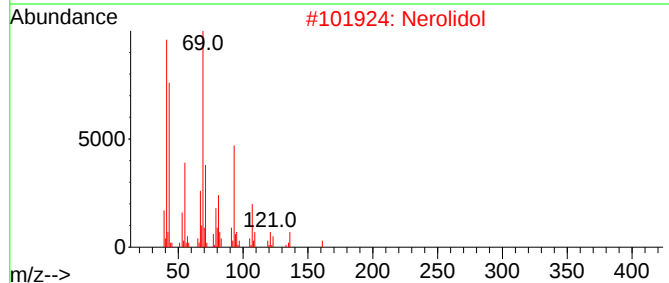
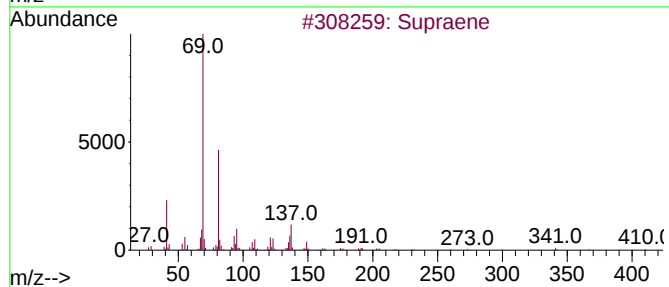
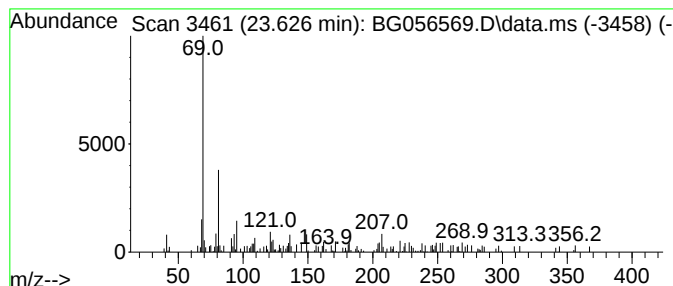
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Peak Number 4 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.626	2.29 ng	78123	Chrysene-d12	21.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	59
2			Nerolidol	222	C15H26O	000142-50-7	53
3			Cyclopropanecarboxylic acid, 4-i...	204	C13H16O2	1000331-01-9	53
4			Geranyl formate	182	C11H18O2	000105-86-2	50
5			(2E,6E,10E)-3,7,11,15-Tetramethy...	318	C21H34O2	125456-63-5	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanol, 2,4...	5.300	16.7	ng	153097	1	8.268	183689	20.0
Tetradecanoic acid	18.473	3.1	ng	88029	4	17.627	565968	20.0
1-Hexacosene	21.493	3.7	ng	127614	5	21.916	682258	20.0
Supraene	23.626	2.3	ng	78123	5	21.916	682258	20.0