LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110222\
Data File : BG055412.D
Acq On : 2 Nov 2022 12:38
Operator : CG/JU
Sample : N5383-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
256317-8

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-BG110122.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055412.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.279	334	339	347	rBV	25351	40141	1.88%	0.464%
2	5.766	416	422	432	rBV	195832	316306	14.79%	3.656%
3	7.388	691	698	712	rBV	126265	224884	10.51%	2.599%
4	8.240	836	843	850	rBV	88469	146477	6.85%	1.693%
5	9.415	1035	1043	1059	rBV	289534	507635	23.73%	5.867%
6	10.813	1274	1281	1301	rBV	83757	162564	7.60%	1.879%
7	11.072	1316	1325	1332	rBV	133586	232406	10.87%	2.686%
8	13.481	1728	1735	1750	rBV	876795	1370980	64.09%	15.844%
9	14.856	1962	1969	1977	rVB	248655	371612	17.37%	4.295%
10	16.336	2215	2221	2237	rBV	739746	1141708	53.38%	13.195%
11	17.594	2428	2435	2441	rBV	319534	481557	22.51%	5.565%
12	18.217	2536	2541	2549	rBV	18987	25271	1.18%	0.292%
13	18.446	2574	2580	2587	rBV	43745	76827	3.59%	0.888%
14	19.697	2789	2793	2797	rBV3	21221	29750	1.39%	0.344%
15	20.167	2867	2873	2878	rBV	1541141	2139024	100.00%	24.720%
16	20.931	3000	3003	3007	rVB	19131	21718	1.02%	0.251%
17	21.477	3088	3096	3107	rBV4	33354	116346	5.44%	1.345%
18	21.859	3155	3161	3171	rVB2	324935	534091	24.97%	6.172%
19	22.012	3183	3187	3192	rVB2	17738	25384	1.19%	0.293%
20	22.641	3289	3294	3301	rVB	16749	26516	1.24%	0.306%
21	23.358	3412	3416	3422	rVB3	12708	21955	1.03%	0.254%
22	23.557	3445	3450	3459	rVB	45131	82585	3.86%	0.954%
23	25.238	3724	3736	3749	rVB2	191198	557131	26.05%	6.439%

Sum of corrected areas: 8652868

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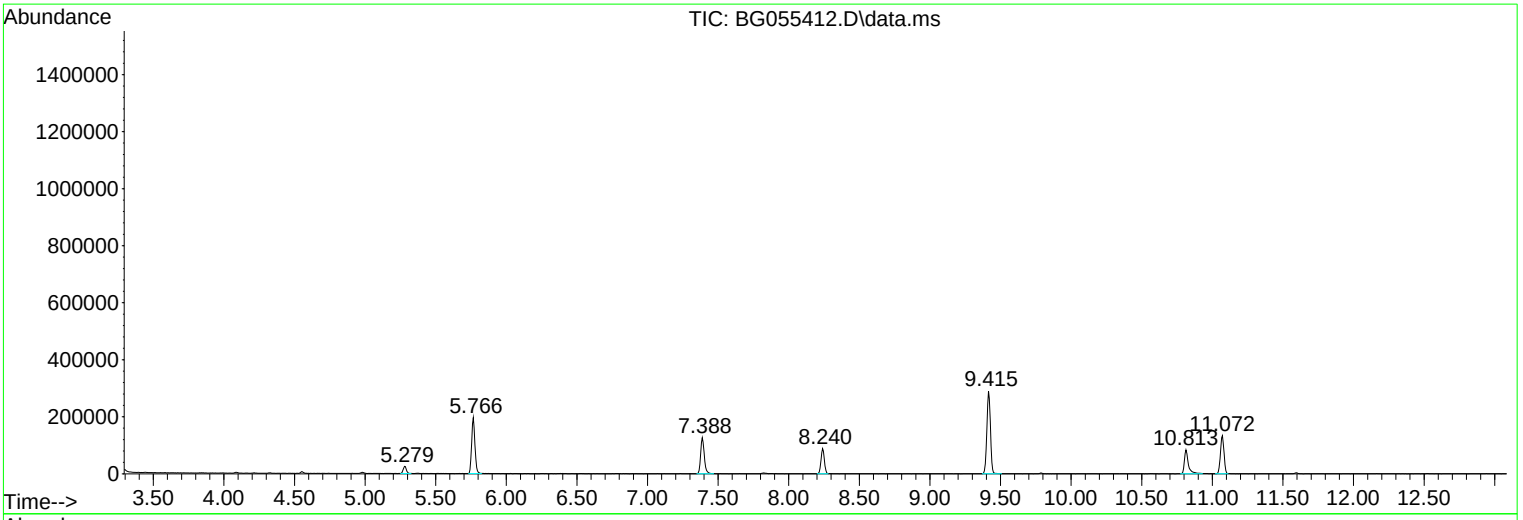
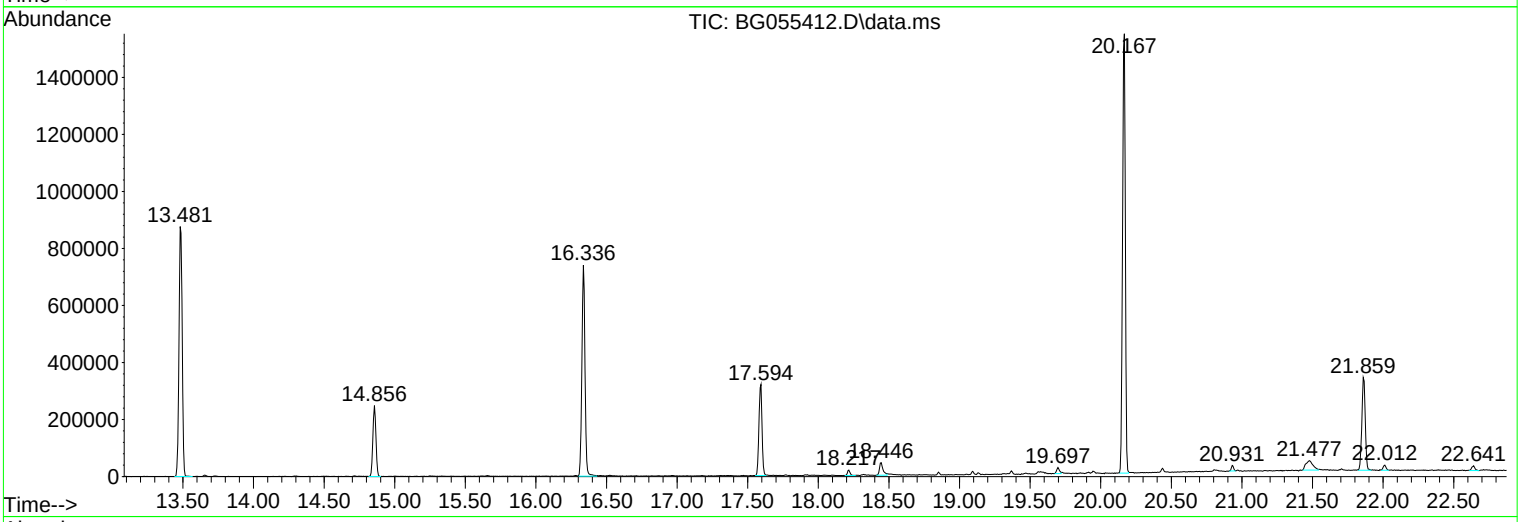
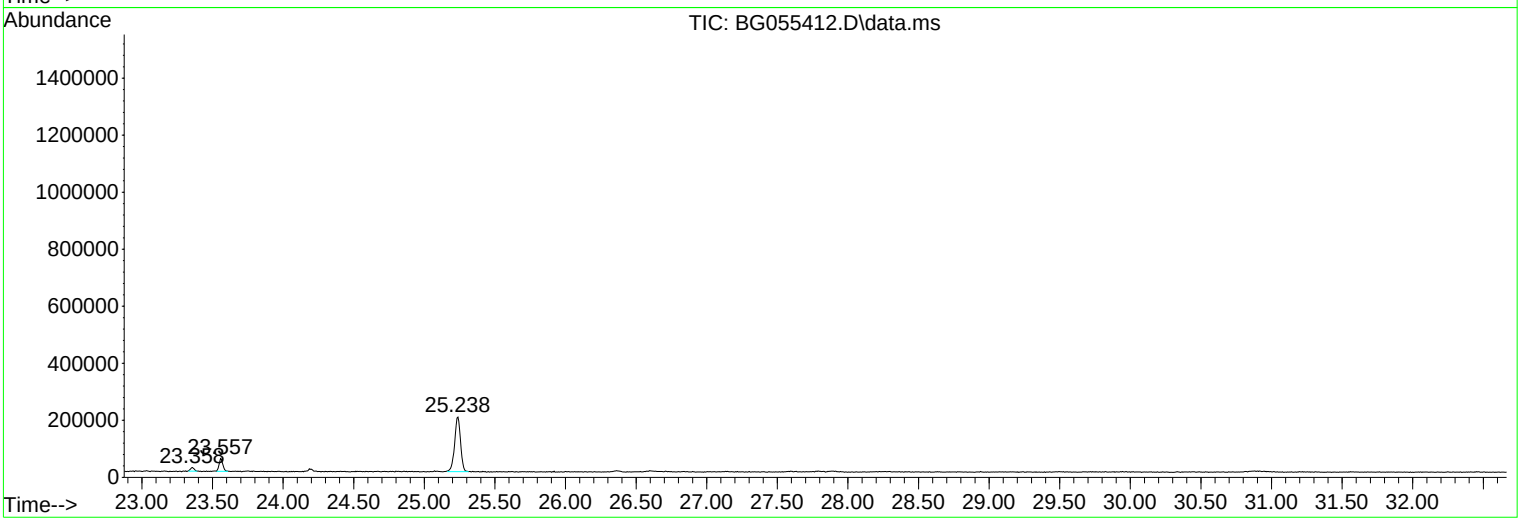
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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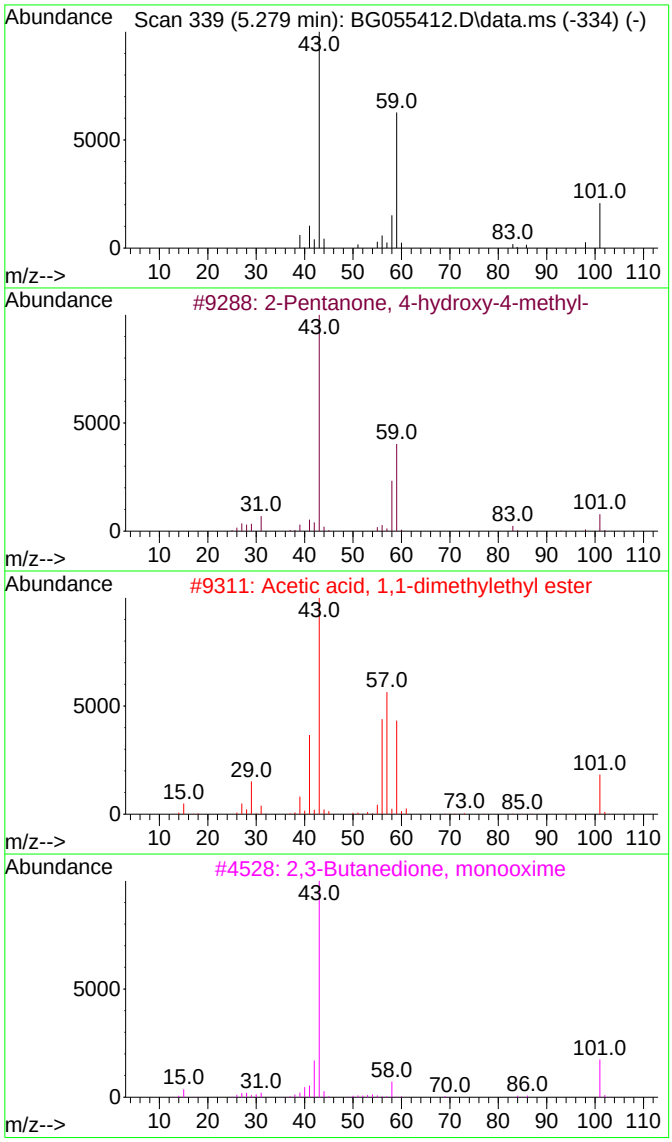
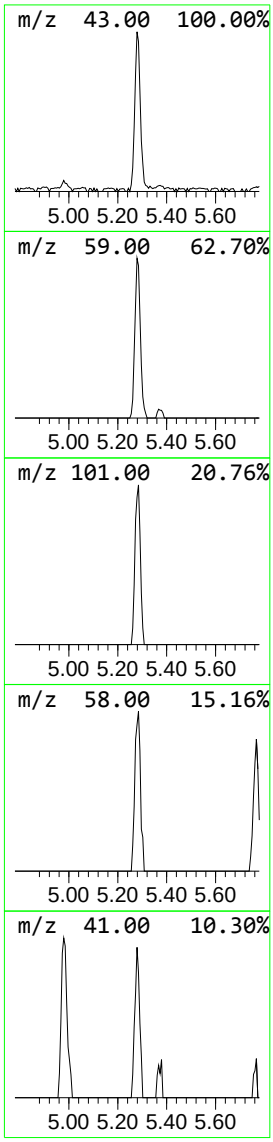
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.279	5.48 ng	40141	1,4-Dichlorobenzene-d4	8.240

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	40
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
4	3-Hexanol	102	C6H14O	000623-37-0	33
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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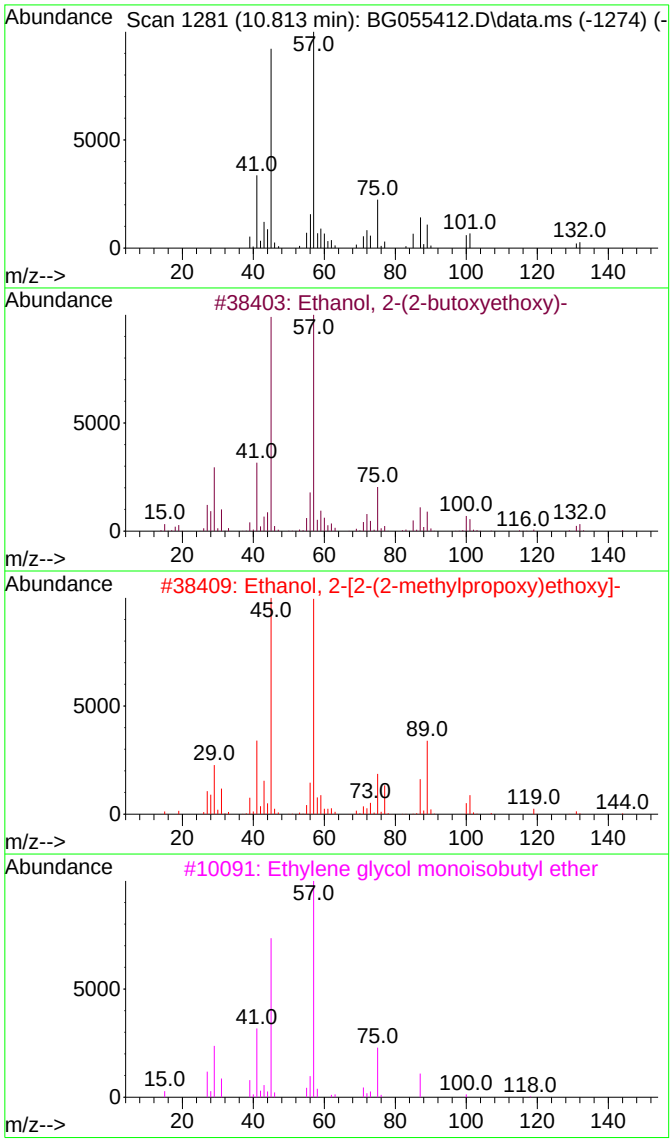
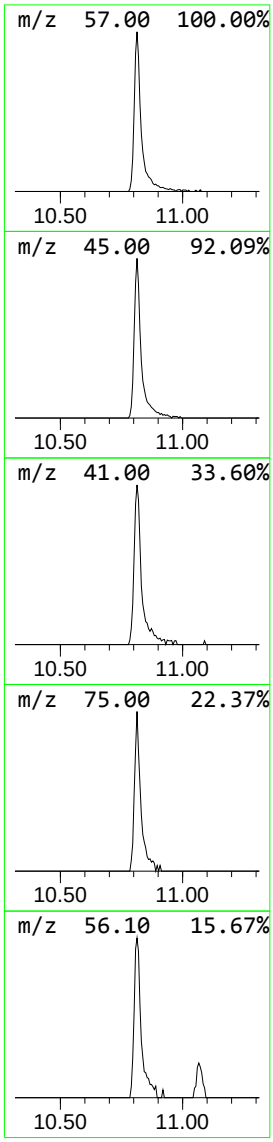
****
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.813	13.99 ng	162564	Naphthalene-d8	11.072

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4	Methoxyacetic acid, 2-butyl ester	146	C7H14O3	070159-90-9	50
5	Di-sec-Butyl ether	130	C8H18O	006863-58-7	50





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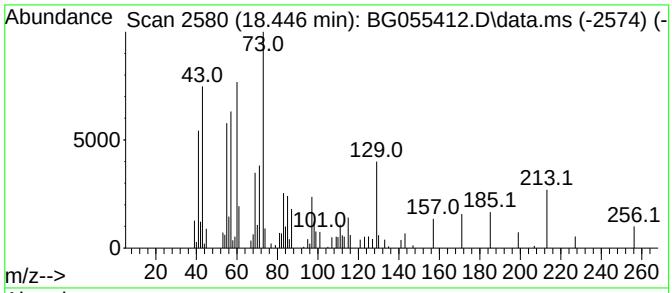
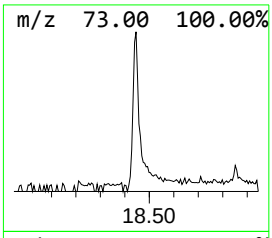
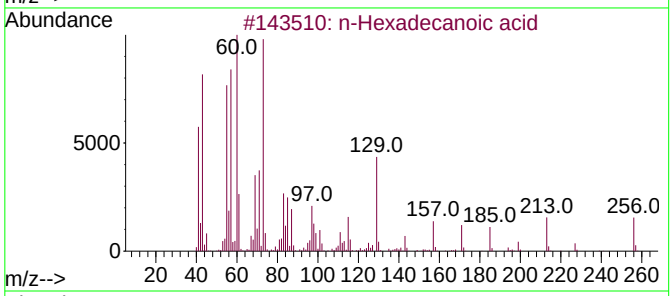
Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

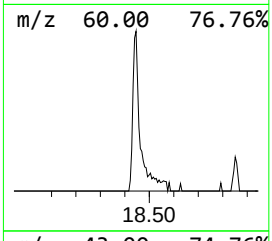
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.446	3.19 ng	76827	Phenanthrene-d10	17.594

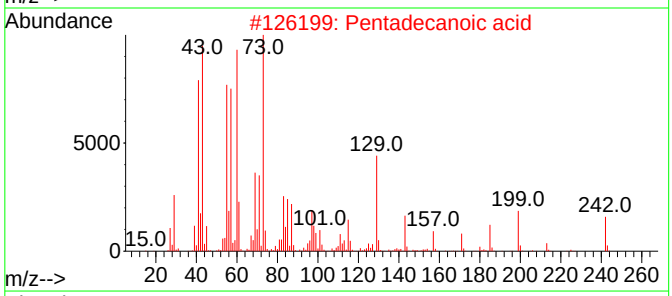
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	n-Decanoic acid	172	C10H20O2	000334-48-5	52
5	Tridecanoic acid	214	C13H26O2	000638-53-9	50

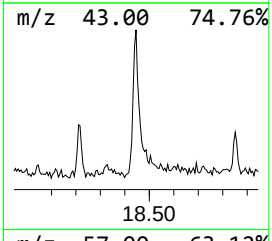


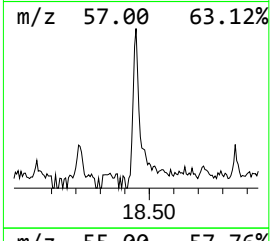


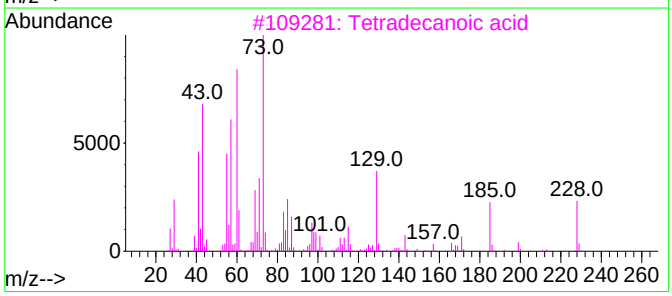


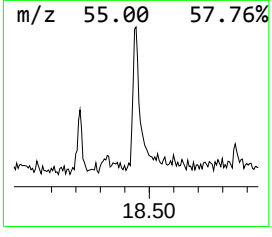












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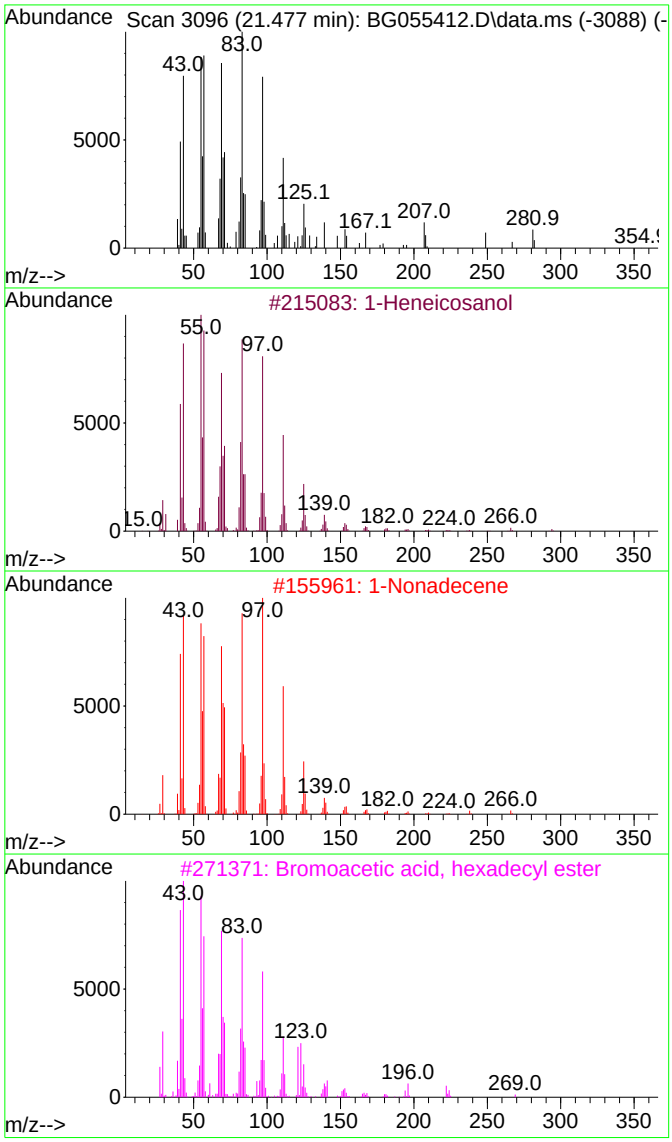
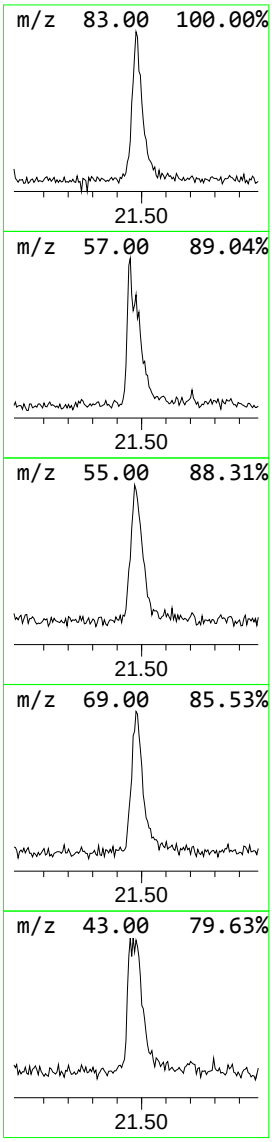
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.477	4.36 ng	116346	Chrysene-d12	21.859

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	91
2	1-Nonadecene	266	C19H38	018435-45-5	91
3	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
4	n-Heptadecanol-1	256	C17H36O	001454-85-9	90
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	90





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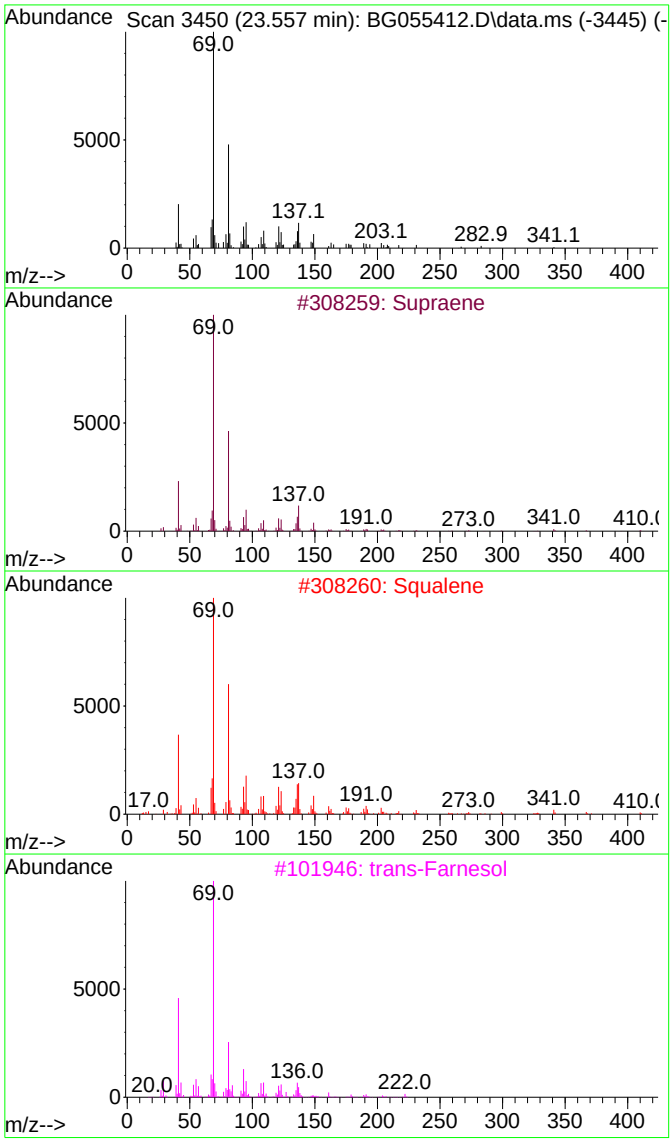
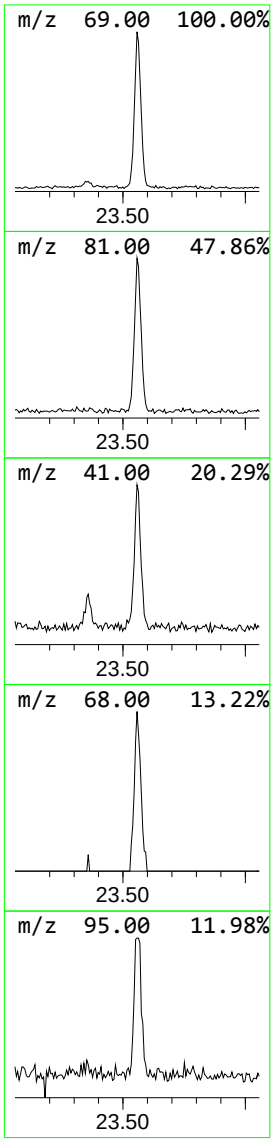
****

Peak Number 5 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.557	2.96 ng	82585	Perylene-d12	25.232

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	Squalene	410	C30H50	000111-02-4	83
3	trans-Farnesol	222	C15H26O	000106-28-5	80
4	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
5	3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	59





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	5.279	5.5	ng	40141	1	8.240	146477	20.0
Ethanol, 2-(2-b...	10.813	14.0	ng	162564	2	11.072	232406	20.0
n-Hexadecanoic ...	18.446	3.2	ng	76827	4	17.594	481557	20.0
1-Heneicosanol	21.477	4.4	ng	116346	5	21.859	534091	20.0
Supraene	23.557	3.0	ng	82585	6	25.232	557131	20.0