LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051050.D
Acq On : 15 Nov 2021 20:46
Operator : CG/JU
Sample : M4674-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MF-WATER-COMP

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-BG111321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG051050.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.759	379	386	396	rBV	335258	556847	19.22%	4.537%
2	7.369	652	660	672	rBV	224396	416185	14.37%	3.391%
3	8.221	799	805	817	rBV	151447	268937	9.28%	2.191%
4	9.402	997	1006	1015	rBV	507909	940923	32.48%	7.667%
5	10.289	1150	1157	1162	rBV2	16110	33249	1.15%	0.271%
6	10.801	1238	1244	1256	rBV	79329	155393	5.36%	1.266%
7	11.053	1279	1287	1295	rBV	218113	401771	13.87%	3.274%
8	13.474	1689	1699	1707	rBV	1327213	2083321	71.91%	16.976%
9	14.849	1925	1933	1941	rVB	380818	605006	20.88%	4.930%
10	16.341	2180	2187	2199	rVB	870785	1400163	48.33%	11.409%
11	17.598	2394	2401	2414	rVB	463475	737826	25.47%	6.012%
12	18.227	2503	2508	2517	rBV	25694	35826	1.24%	0.292%
13	18.450	2541	2546	2556	rBV	74063	122145	4.22%	0.995%
14	19.708	2755	2760	2770	rBV3	27822	53476	1.85%	0.436%
15	20.190	2835	2842	2847	rBV	2080714	2896985	100.00%	23.606%
16	21.488	3058	3063	3076	rVB3	79899	172122	5.94%	1.403%
17	21.893	3126	3132	3140	rVB	370574	650686	22.46%	5.302%
18	23.615	3421	3425	3431	rVB	38613	77118	2.66%	0.628%
19	25.301	3703	3712	3725	rVB3	216154	664259	22.93%	5.413%

Sum of corrected areas: 12272238

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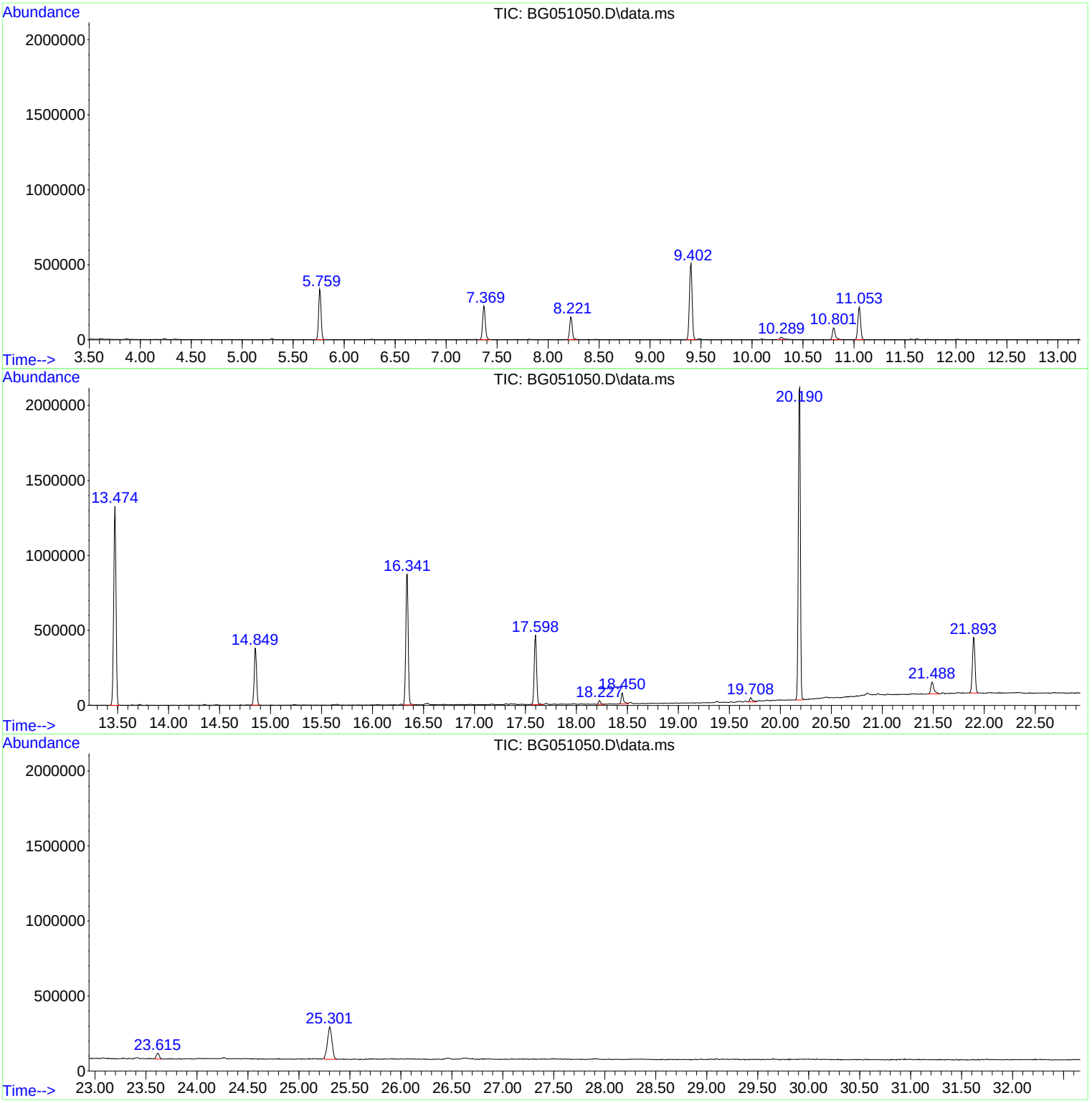
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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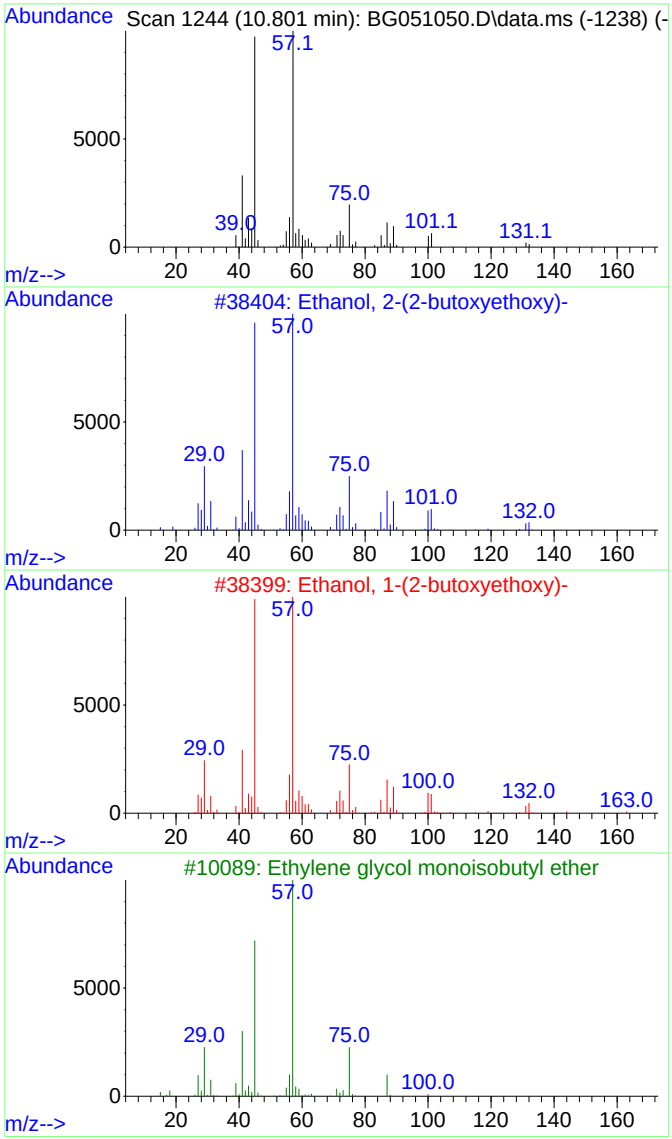
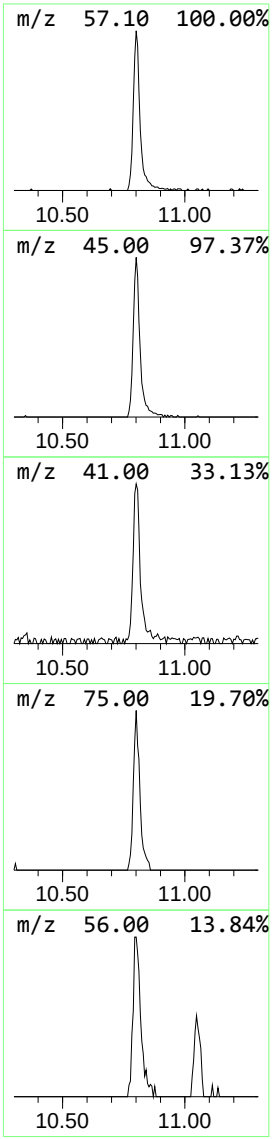
Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.801	7.74 ng	155393	Naphthalene-d8	11.053

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4	Di-sec-Butyl ether	130	C8H18O	006863-58-7	50
5	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50





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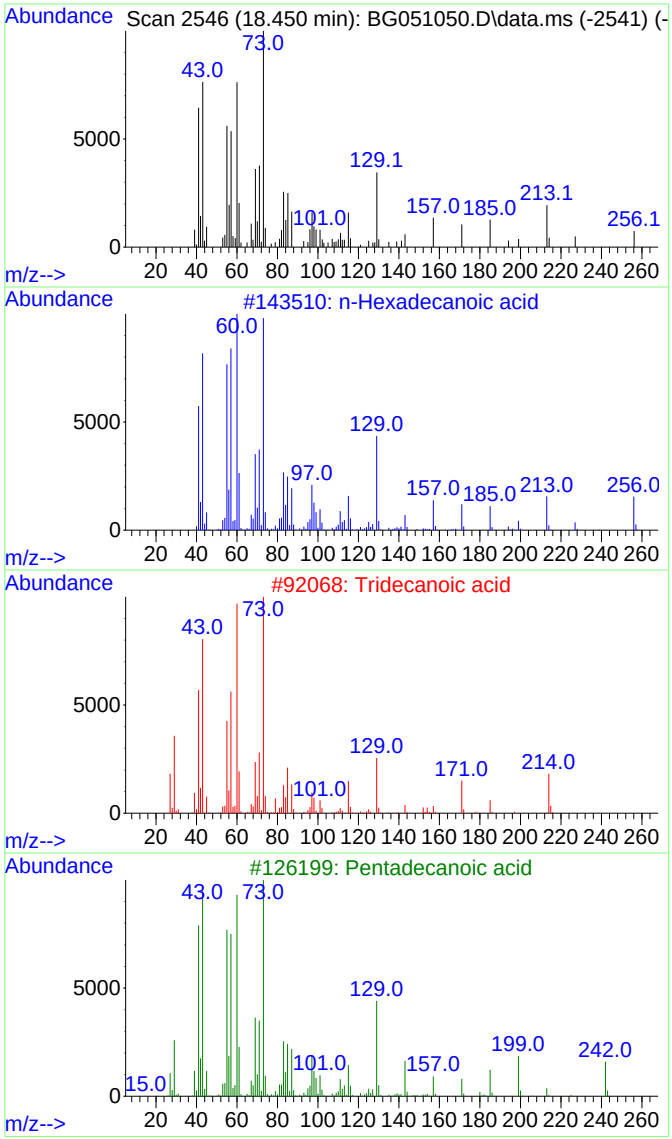
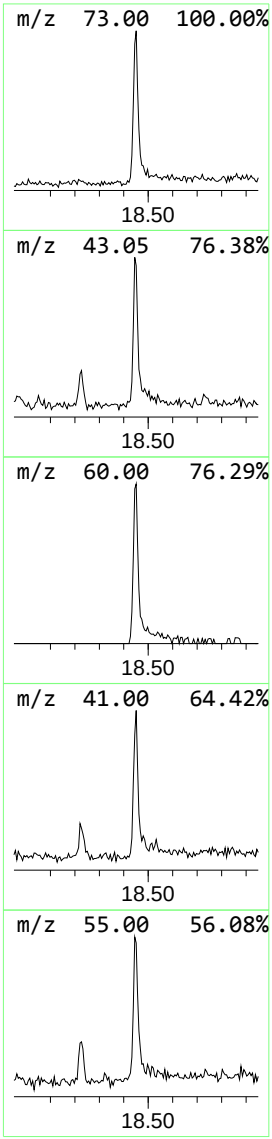
Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.450	3.31 ng	122145	Phenanthrene-d10	17.599

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	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	50





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BNA_G
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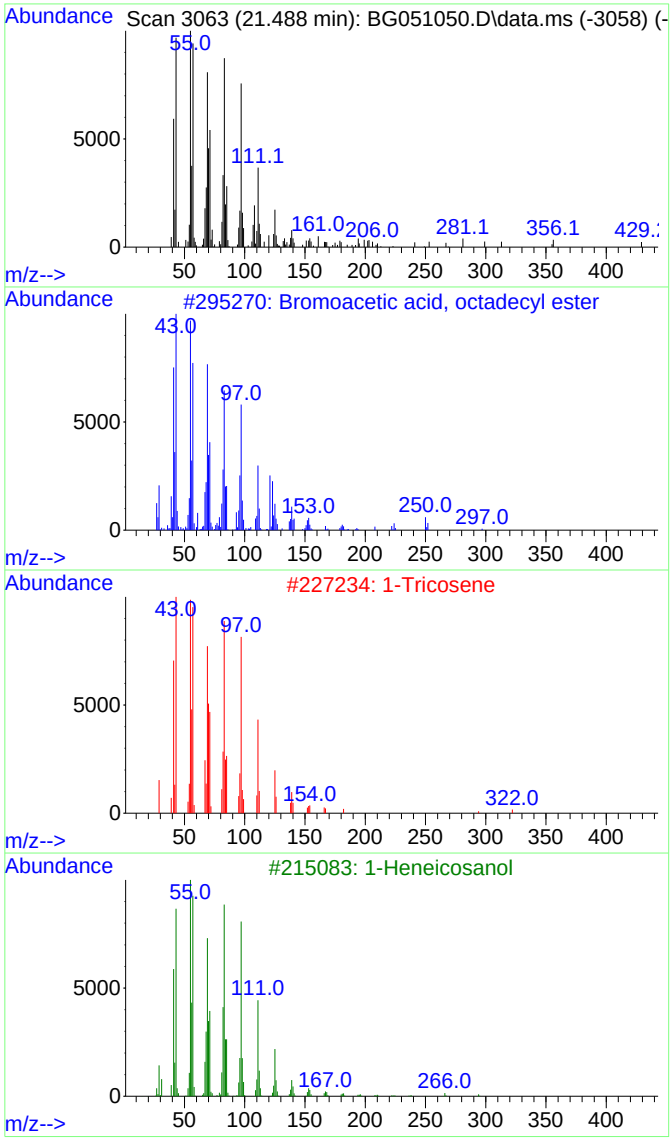
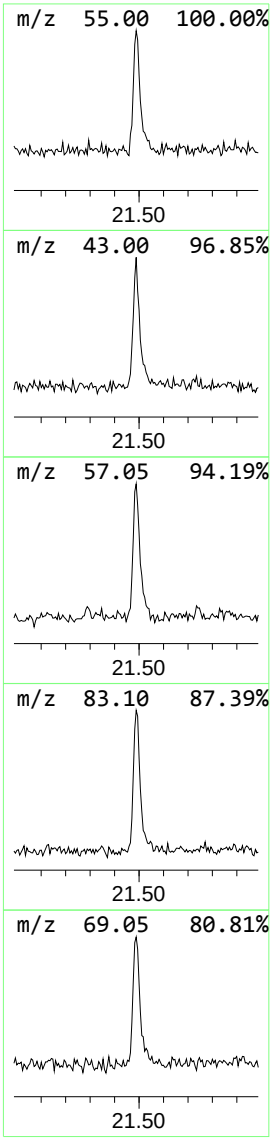
Peak Number 3 Bromoacetic acid, octadecyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.488	5.29 ng	172122	Chrysene-d12	21.894

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	94
2	1-Tricosene	322	C23H46	018835-32-0	93
3	1-Heneicosanol	312	C21H44O	015594-90-8	93
4	Behenic alcohol	326	C22H46O	000661-19-8	93
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	93





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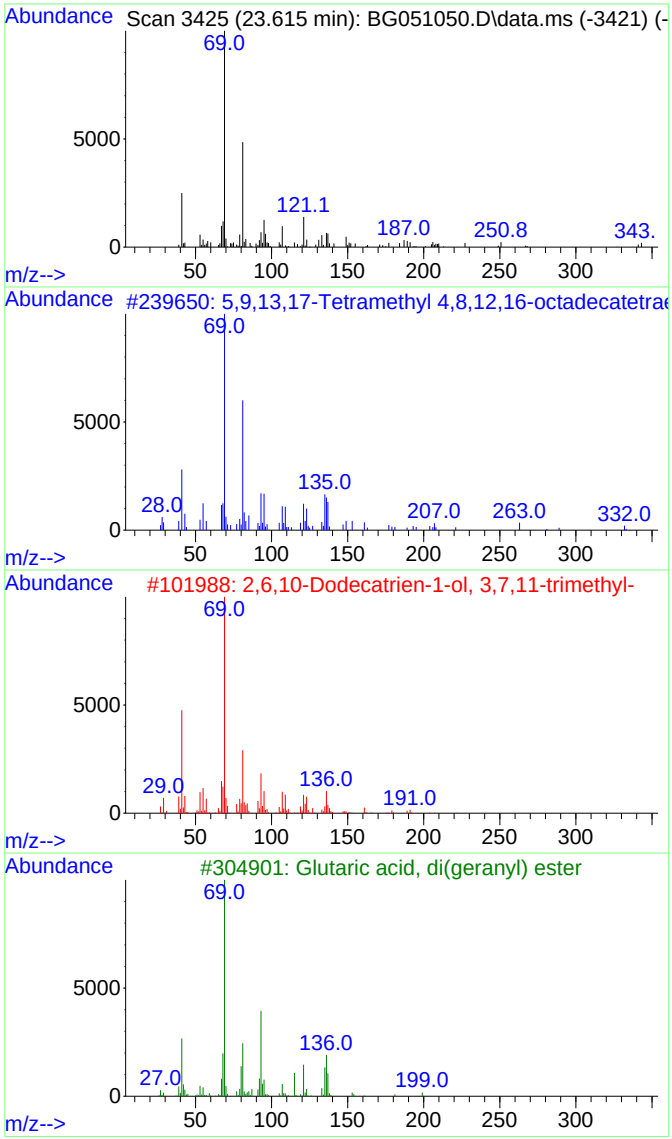
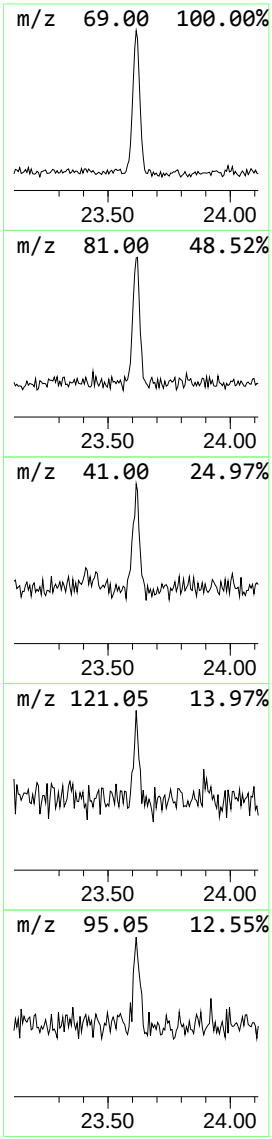
Peak Number 4 5,9,13,17-Tetramethyl 4,8,1... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.615	2.32 ng	77118	Perylene-d12	25.301

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,9,13,17-Tetramethyl 4,8,12,16-...	332	C22H36O2	1000432-37-9	64
2	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	56
3	Glutaric acid, di(geranyl) ester	404	C25H40O4	1000405-03-0	56
4	4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	53
5	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	50





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Ethanol, 2-(2-b...	10.801	7.7	ng	155393	2	11.053	401771	20.0
n-Hexadecanoic ...	18.450	3.3	ng	122145	4	17.599	737826	20.0
Bromoacetic aci...	21.488	5.3	ng	172122	5	21.894	650686	20.0
5,9,13,17-Tetra...	23.615	2.3	ng	77118	6	25.301	664259	20.0