LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111222\
Data File : BG055592.D
Acq On : 12 Nov 2022 16:36
Operator : CG/JU
Sample : N5431-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221177-COMP-12-MODIFIED-ELUTRIATE

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-BG110922.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055592.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.323	3	6	25	rVB	724314	1090826	27.65%	6.180%
2	4.704	236	241	247	rBV	28948	41288	1.05%	0.234%
3	5.321	338	346	354	rBV	56659	88474	2.24%	0.501%
4	5.791	419	426	435	rBV	453903	715482	18.13%	4.054%
5	7.401	692	700	708	rBV	308611	533602	13.52%	3.023%
6	8.265	841	847	858	rBV	222289	382596	9.70%	2.168%
7	9.440	1039	1047	1057	rVB	543668	971624	24.63%	5.505%
8	11.097	1321	1329	1338	rVB	312716	556081	14.09%	3.151%
9	13.517	1733	1741	1748	rBV	1489979	2315193	58.68%	13.117%
10	14.886	1967	1974	1981	rVB	555331	850209	21.55%	4.817%
11	16.367	2218	2226	2236	rBV	1479270	2190485	55.52%	12.411%
12	17.624	2433	2440	2447	rBV	714000	1134569	28.76%	6.428%
13	18.488	2582	2587	2596	rBV	80855	126745	3.21%	0.718%
14	19.745	2796	2801	2810	rBV2	57041	91071	2.31%	0.516%
15	20.215	2875	2881	2887	rBV	3011108	3945436	100.00%	22.354%
16	21.925	3166	3172	3179	rVB2	748172	1253177	31.76%	7.100%
17	25.350	3744	3755	3769	rVB2	435200	1362954	34.55%	7.722%

Sum of corrected areas: 17649812

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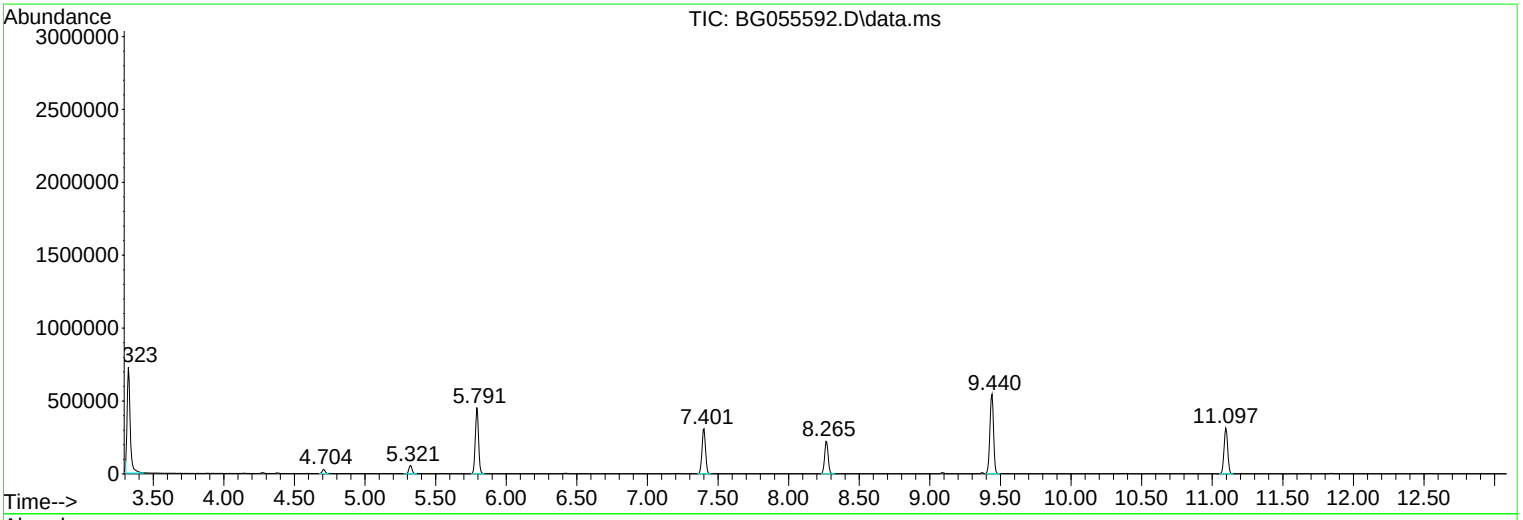
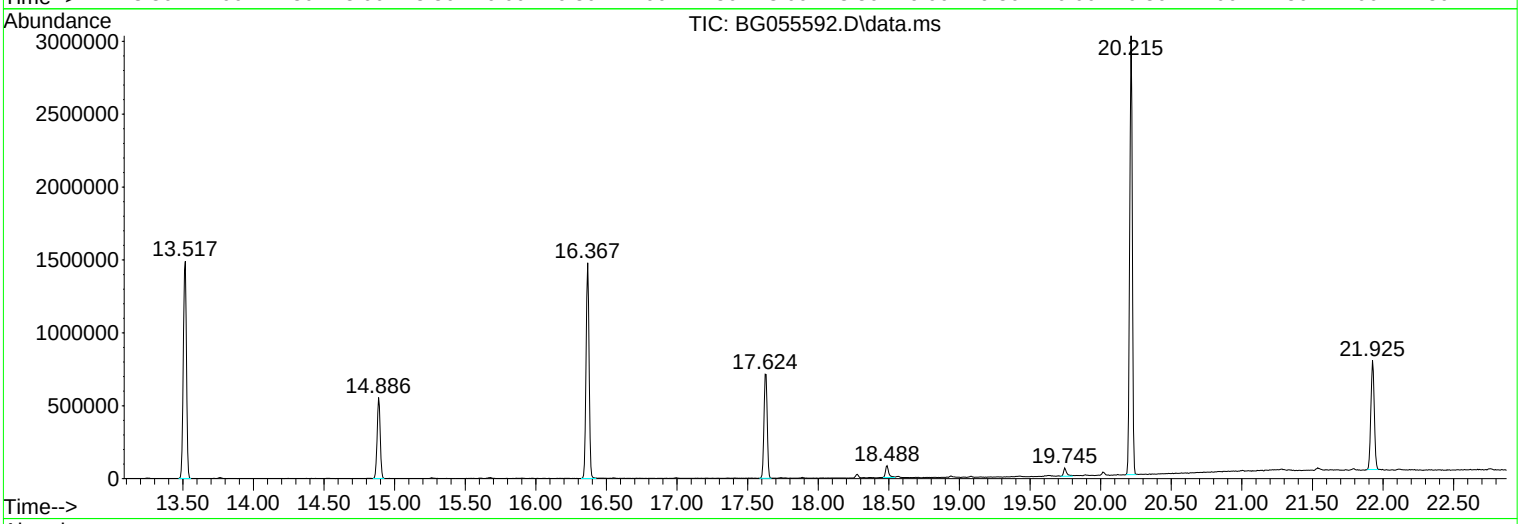
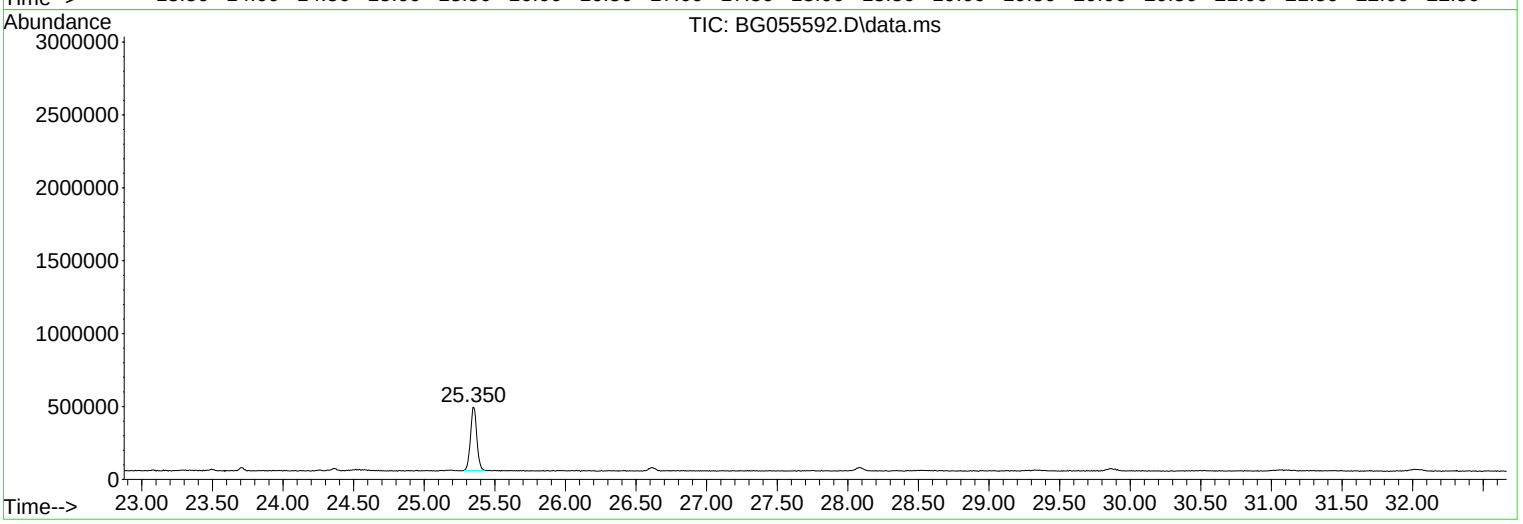
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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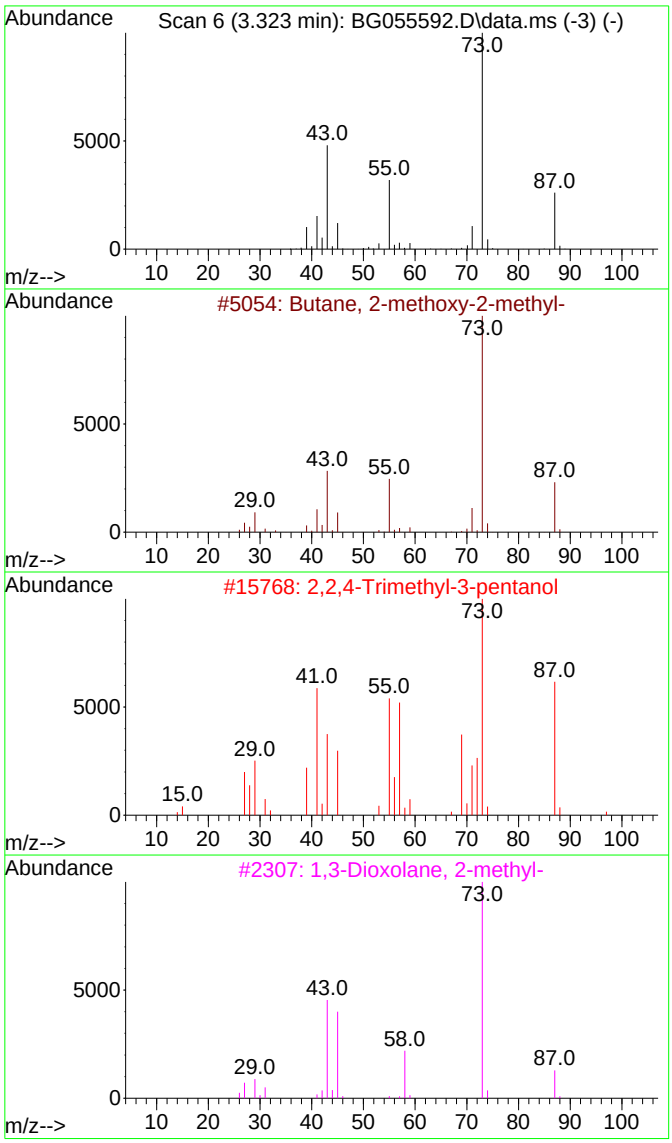
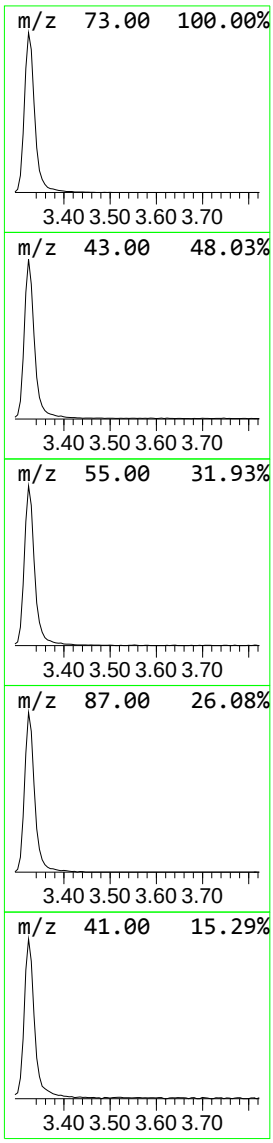
****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.323	57.02 ng	1090830	1,4-Dichlorobenzene-d4	8.270

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





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Instrument :
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ClientSampleId :
20221177-COMP-12-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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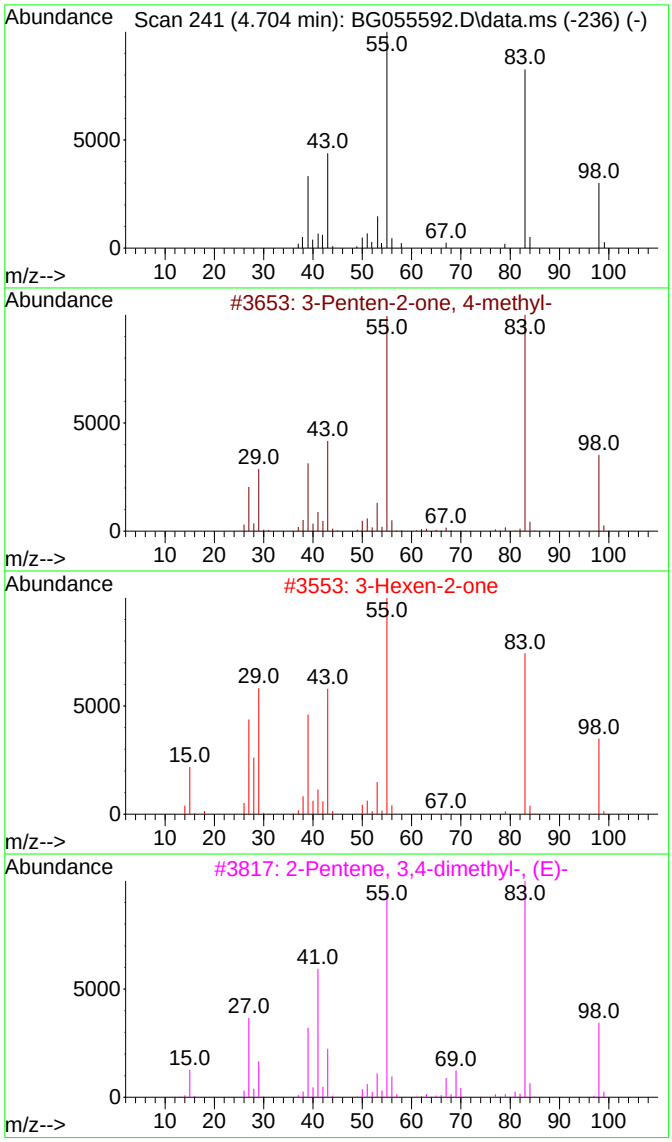
TIC Integration Parameters: LSCINT.P

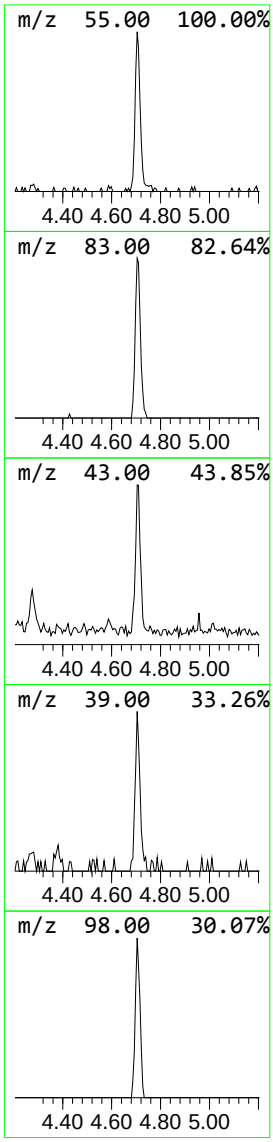
****

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.704	2.16 ng	41288	1,4-Dichlorobenzene-d4	8.270

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	86





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Operator : CG/JU
Sample : N5431-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221177-COMP-12-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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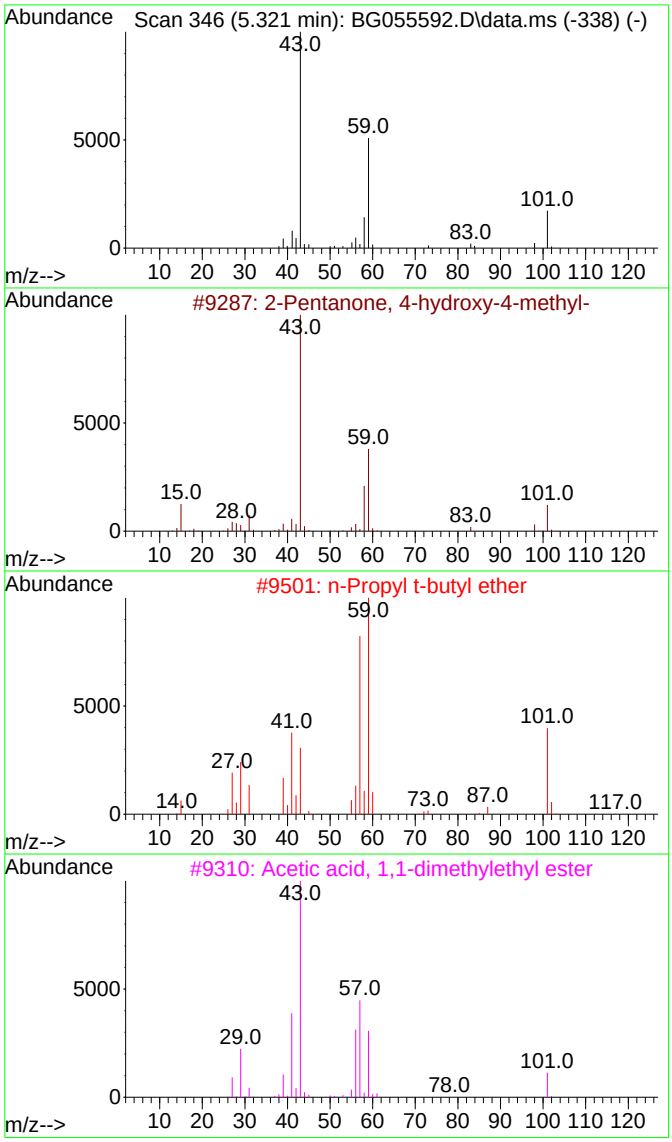
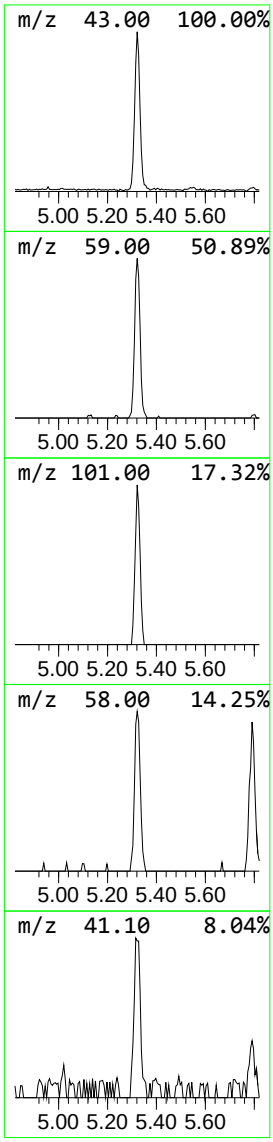
****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.321	4.62 ng	88474	1,4-Dichlorobenzene-d4	8.270

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	Guanidine	59	CH5N3	000113-00-8	9





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Instrument :
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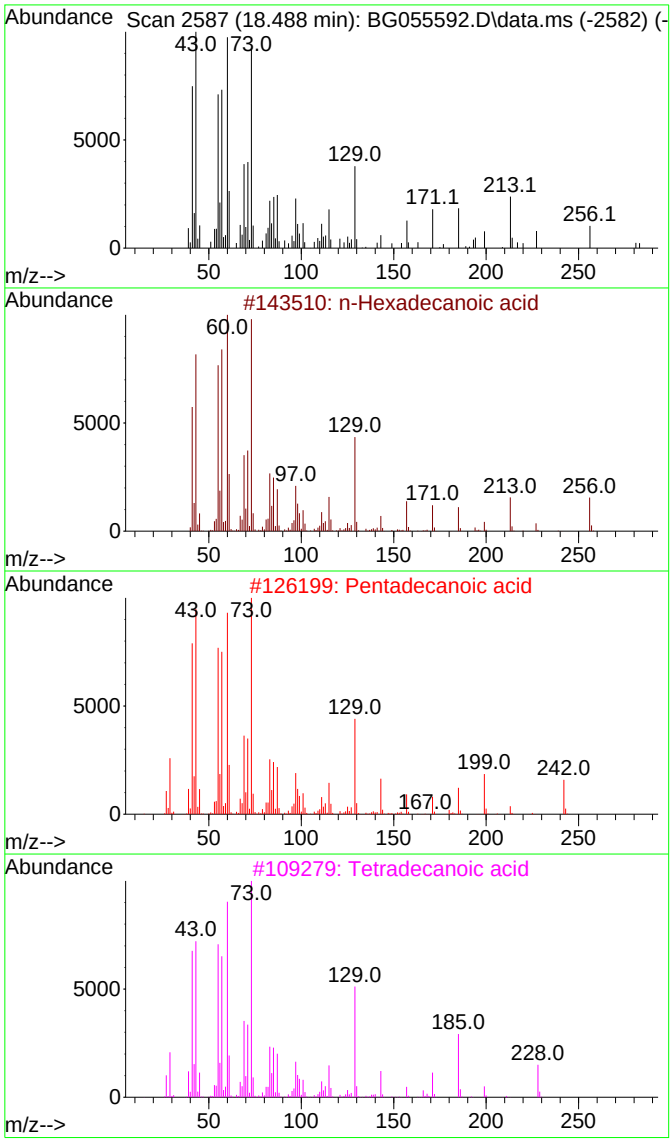
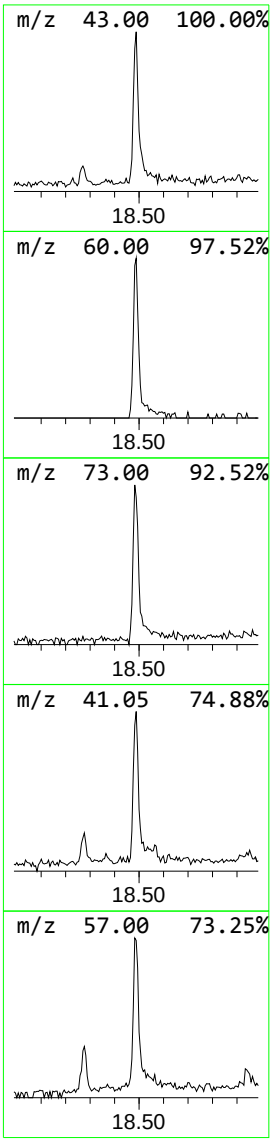
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.488	2.23 ng	126745	Phenanthrene-d10	17.630

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	60
5	Nonanoic acid	158	C9H18O2	000112-05-0	43





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	3.323	57.0	ng	1090830	1	8.270	382596	20.0
3-Penten-2-one,...	4.704	2.2	ng	41288	1	8.270	382596	20.0
2-Pentanone, 4-...	5.321	4.6	ng	88474	1	8.270	382596	20.0
n-Hexadecanoic ...	18.488	2.2	ng	126745	4	17.630	1134570	20.0