LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080621\
Data File : BP006554.D
Acq On : 06 Aug 2021 23:55
Operator : CG/JU
Sample : M3279-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 20210580-COM-3

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_P\Methods\8270E-BP080321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP006554.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.905	304	309	318	rVB	1971151	2731126	28.06%	4.343%
2	5.358	380	386	395	rVB	5070067	7041997	72.36%	11.199%
3	5.970	485	490	498	rVB	398768	585523	6.02%	0.931%
4	6.934	647	654	667	rBV	4623129	7314143	75.16%	11.632%
5	7.752	787	793	802	rVB	849286	1295398	13.31%	2.060%
6	8.911	982	990	1001	rBV	2904949	4700688	48.30%	7.476%
7	10.328	1224	1231	1243	rBV	621207	954098	9.80%	1.517%
8	10.534	1258	1266	1273	rBV	1096551	1782260	18.31%	2.834%
9	13.004	1678	1686	1700	rBV	5270477	7943946	81.63%	12.633%
10	14.381	1909	1920	1927	rBV	1445389	2101089	21.59%	3.341%
11	15.875	2163	2174	2183	rBV	4534416	6601433	67.83%	10.498%
12	17.134	2381	2388	2393	rBV	1696860	2340809	24.05%	3.723%
13	18.040	2537	2542	2550	rBV	305655	450565	4.63%	0.717%
14	19.145	2725	2730	2737	rBV2	80171	173616	1.78%	0.276%
15	19.281	2749	2753	2763	rBV	131022	194839	2.00%	0.310%
16	19.710	2820	2826	2831	rBV	8228858	9731927	100.00%	15.477%
17	20.504	2957	2961	2965	rBV2	167147	191276	1.97%	0.304%
18	20.957	3034	3038	3045	rBV	459614	601751	6.18%	0.957%
19	21.228	3079	3084	3089	rBV	2152830	2635729	27.08%	4.192%
20	21.392	3109	3112	3116	rBV	223697	231448	2.38%	0.368%
21	21.845	3186	3189	3194	rVB	187870	220975	2.27%	0.351%
22	22.328	3268	3271	3276	rVB2	162796	221266	2.27%	0.352%
23	23.557	3473	3480	3494	rVB2	1411633	2834413	29.12%	4.508%

Sum of corrected areas: 62880315

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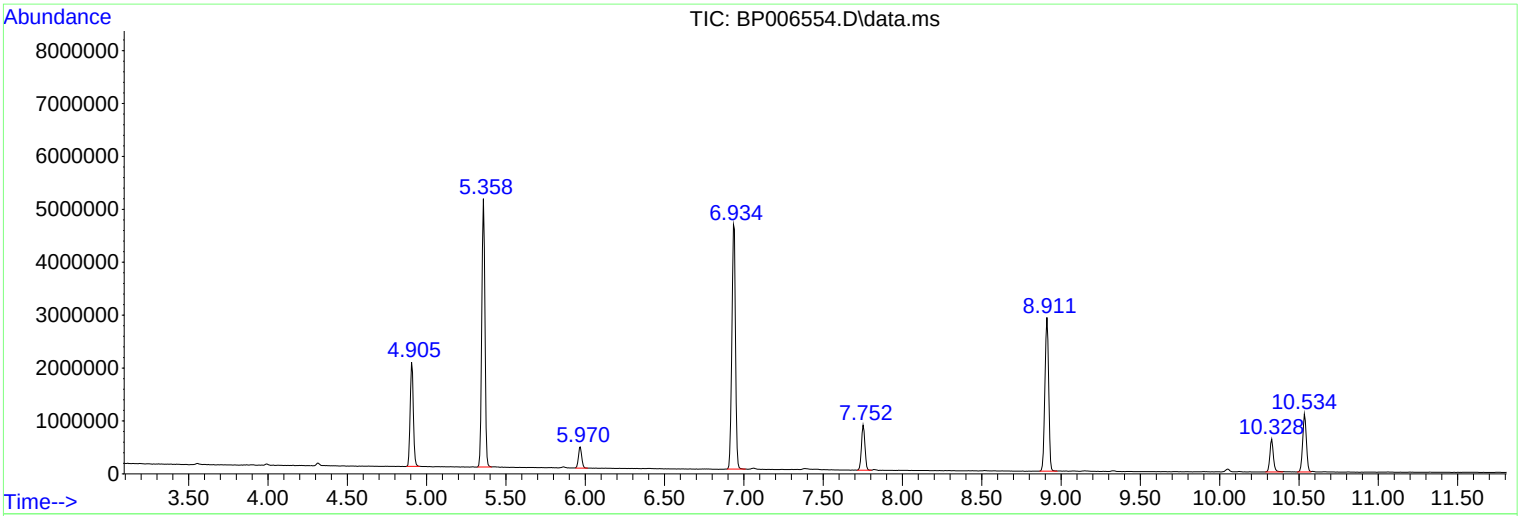
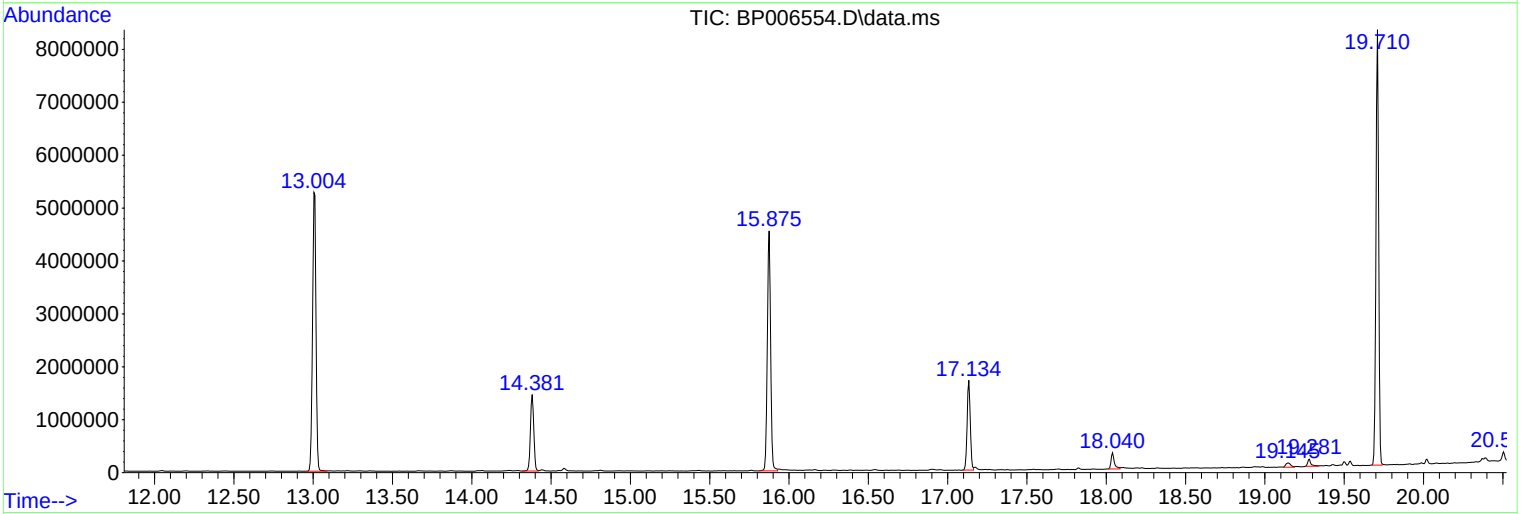
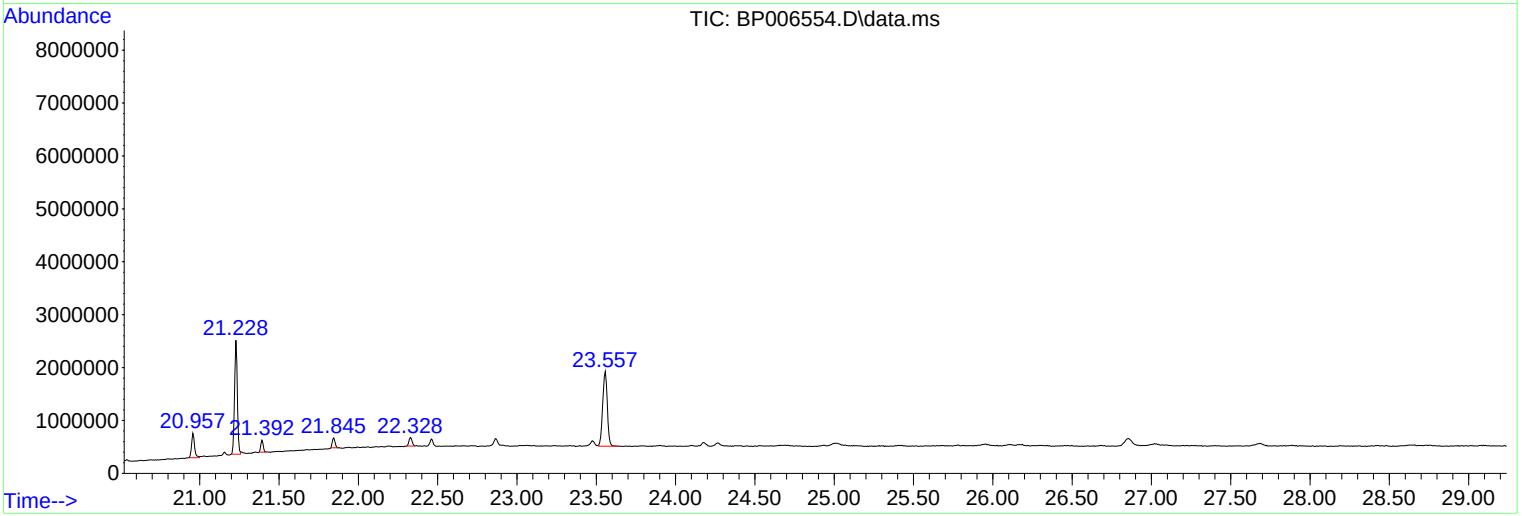
ClientSampleId :
20210580-COM-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.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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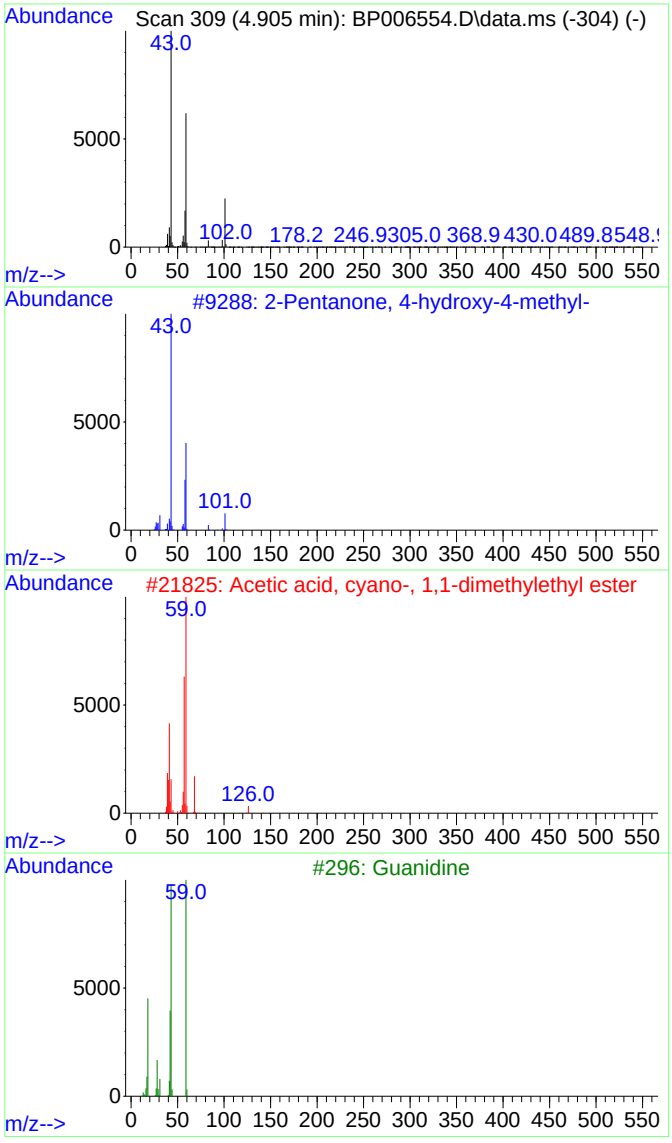
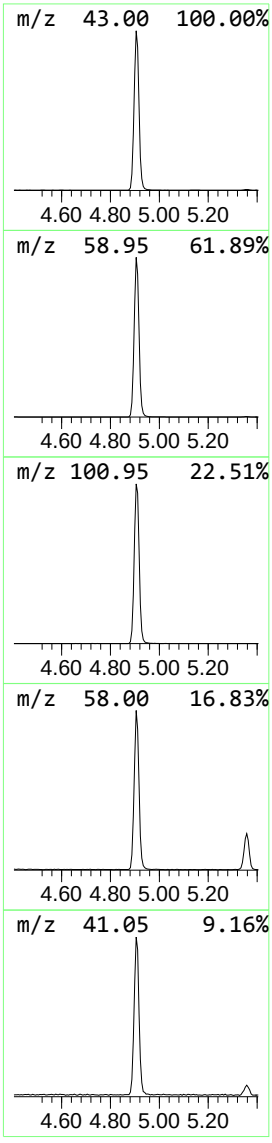
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.905	42.17 ng	2731130	1,4-Dichlorobenzene-d4	7.752

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
3	Guanidine	59	CH5N3	000113-00-8	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Acetone	58	C3H6O	000067-64-1	9





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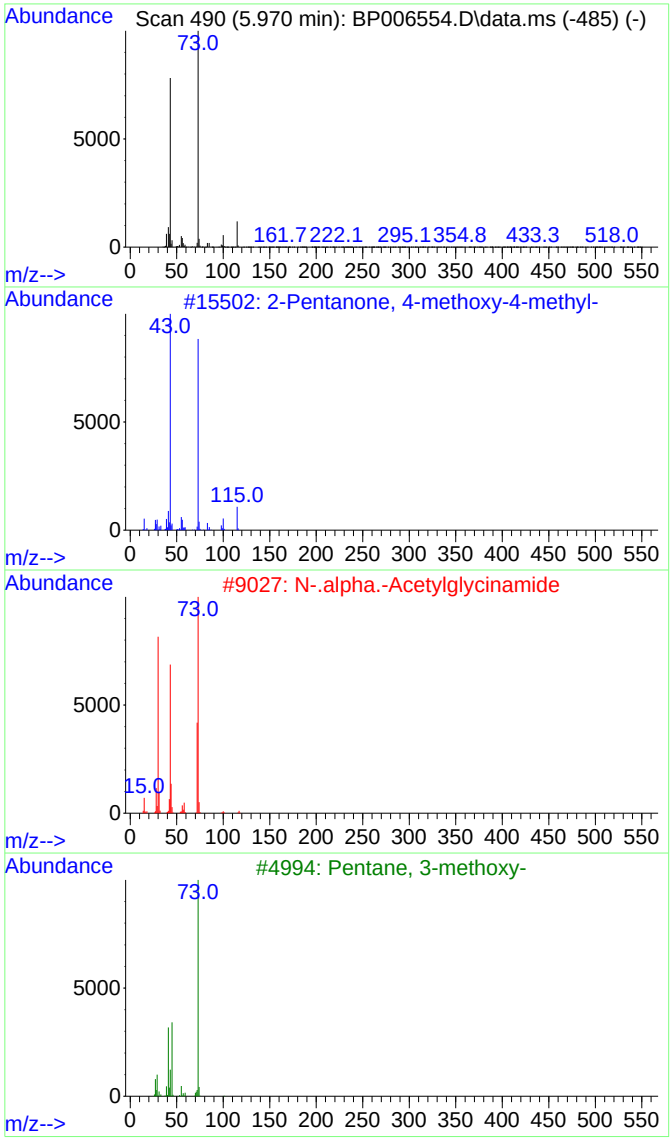
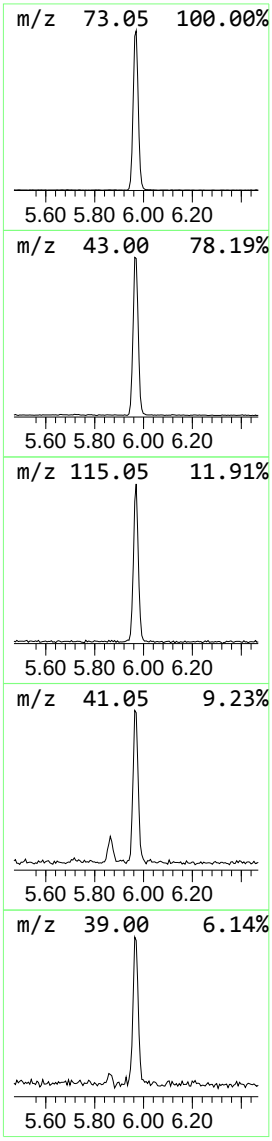
****
Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.970	9.04 ng	585523	1,4-Dichlorobenzene-d4	7.752

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	47
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	10
5	N-Formylmorpholine	115	C5H9NO2	004394-85-8	9





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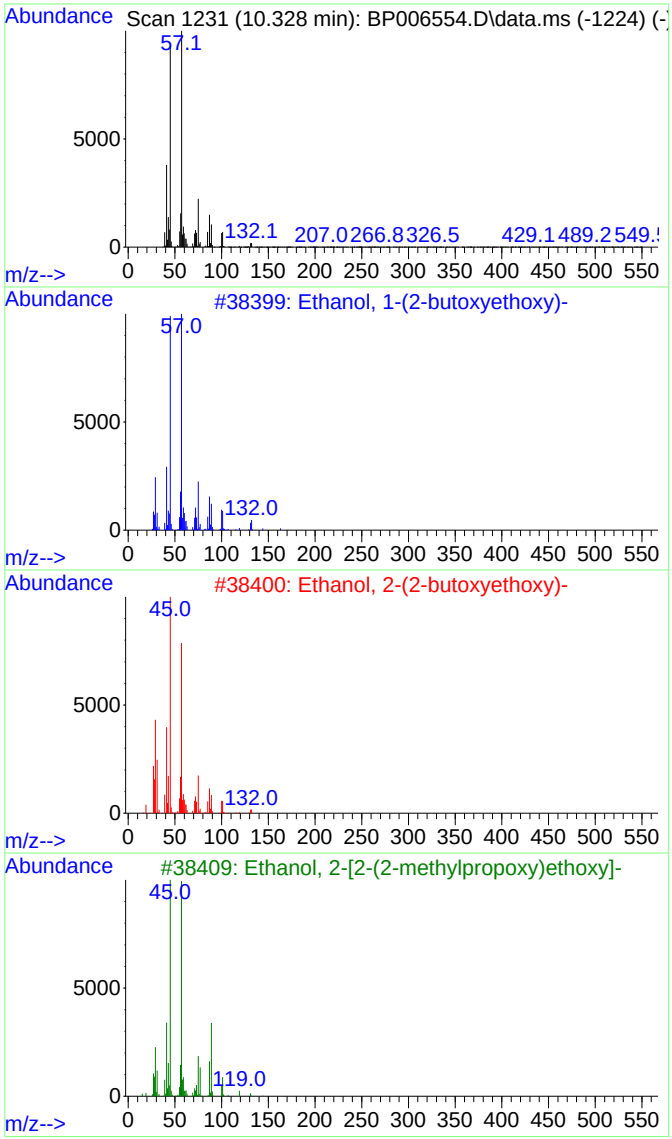
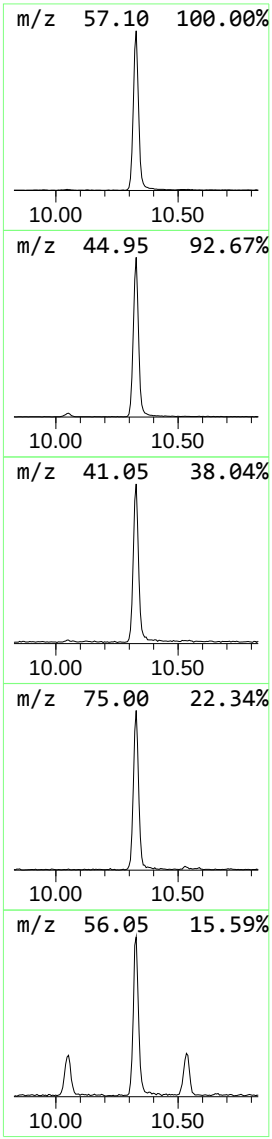
Peak Number 3 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.328	10.71 ng	954098	Naphthalene-d8	10.534

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
2	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	72
4	Di-sec-Butyl ether	130	C8H18O	006863-58-7	50
5	Methoxyacetic acid, 2-butyl ester	146	C7H14O3	070159-90-9	50





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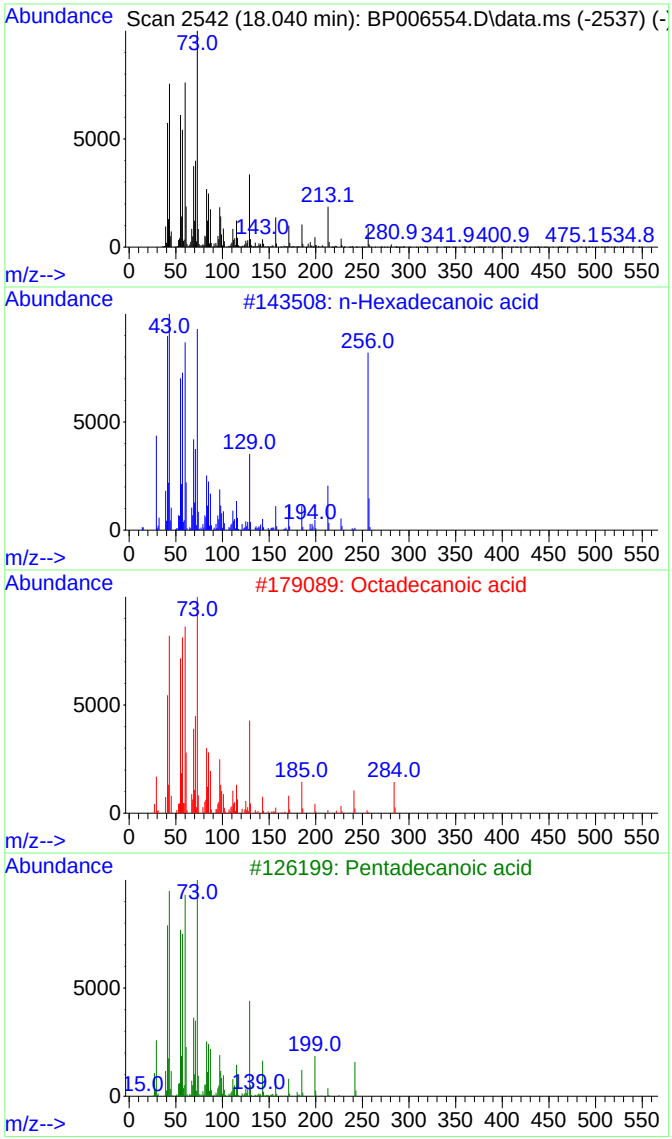
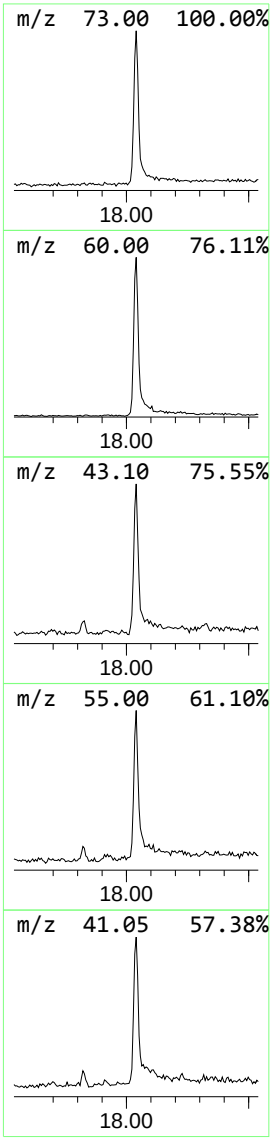
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.040	3.85 ng	450565	Phenanthrene-d10	17.134

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Octadecanoic acid	284	C18H36O2	000057-11-4	76
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5	Dodecanoic acid	200	C12H24O2	000143-07-7	68





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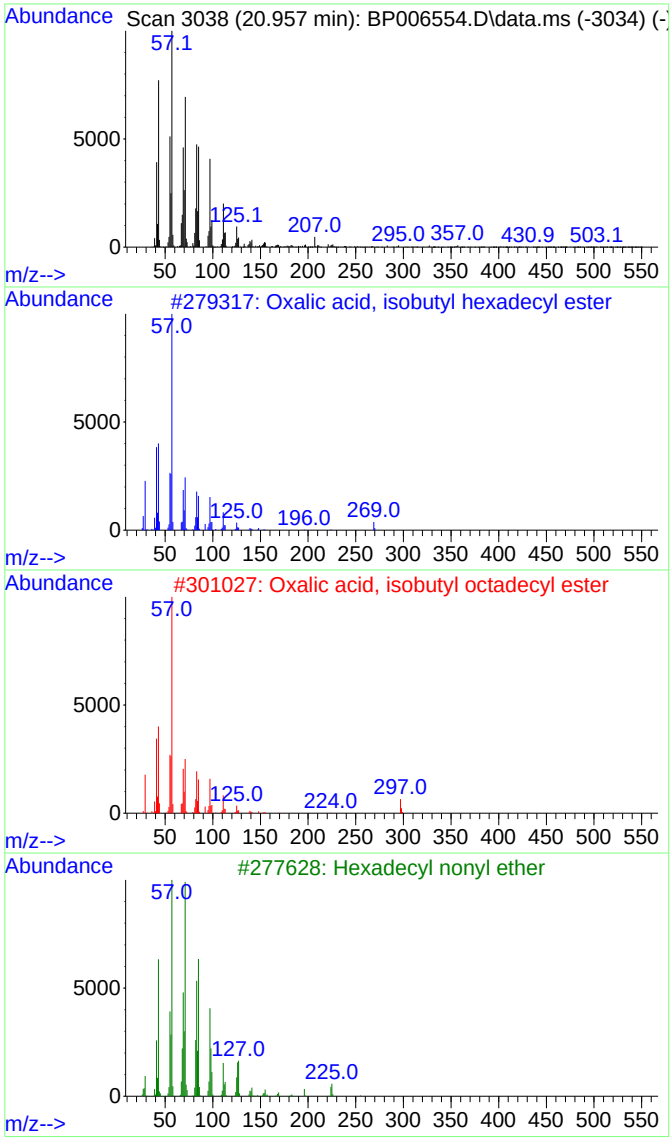
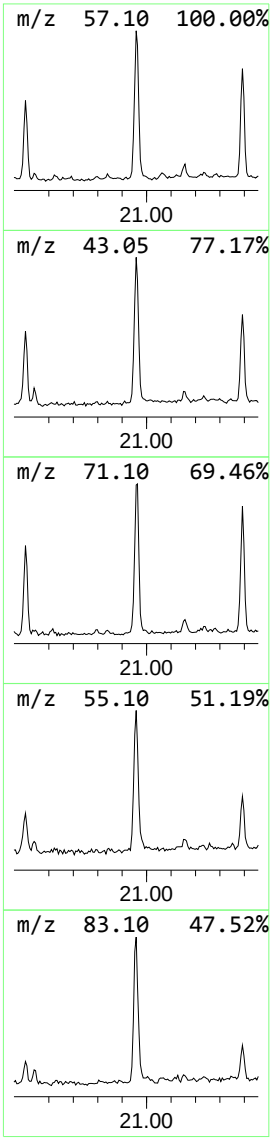
****
Peak Number 5 Oxalic acid, isobutyl hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.957	4.57 ng	601751	Chrysene-d12	21.228

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
2	Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	91
3	Hexadecyl nonyl ether	368	C25H52O	1000406-37-7	90
4	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	90
5	1-Hexacosanol	382	C26H54O	000506-52-5	87





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-...	4.905	42.2	ng	2731130	1	7.752	1295400	20.0
2-Pentanone, 4-...	5.970	9.0	ng	585523	1	7.752	1295400	20.0
Ethanol, 1-(2-b...	10.328	10.7	ng	954098	2	10.534	1782260	20.0
n-Hexadecanoic ...	18.040	3.9	ng	450565	4	17.134	2340810	20.0
Oxalic acid, is...	20.957	4.6	ng	601751	5	21.228	2635730	20.0