LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091322\
Data File : BG054931.D
Acq On : 13 Sep 2022 21:09
Operator : CG/JU
Sample : N4578-41
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CHERRY-HILL-COMP-10

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-BG082522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054931.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.193	319	324	335	rVB	23614	37489	2.06%	0.386%
2	5.675	400	406	418	rBV	428415	712596	39.15%	7.346%
3	7.291	672	681	691	rBV	421547	748433	41.12%	7.715%
4	8.131	818	824	832	rBV	129906	228267	12.54%	2.353%
5	9.312	1016	1025	1035	rBV	243875	450985	24.77%	4.649%
6	10.710	1253	1263	1280	rBV2	38649	84950	4.67%	0.876%
7	10.963	1298	1306	1314	rBV	182034	330983	18.18%	3.412%
8	13.395	1712	1720	1734	rBV	763720	1222829	67.18%	12.606%
9	14.770	1947	1954	1967	rBV	322780	503793	27.68%	5.194%
10	16.263	2201	2208	2226	rBV	573866	969619	53.27%	9.996%
11	16.457	2235	2241	2252	rVB	81388	127254	6.99%	1.312%
12	17.520	2415	2422	2430	rBV	421418	649070	35.66%	6.691%
13	20.117	2858	2864	2874	rBV	1398598	1820340	100.00%	18.766%
14	20.399	2908	2912	2917	rVB	19285	24255	1.33%	0.250%
15	20.893	2993	2996	3000	rBV	31334	37679	2.07%	0.388%
16	21.415	3080	3085	3098	rVB2	68135	129783	7.13%	1.338%
17	21.809	3146	3152	3166	rVB2	390495	700941	38.51%	7.226%
18	21.974	3176	3180	3186	rVB2	35221	50171	2.76%	0.517%
19	22.602	3283	3287	3293	rVB	29225	45280	2.49%	0.467%
20	23.325	3406	3410	3422	rVB2	24354	47793	2.63%	0.493%
21	25.187	3716	3727	3742	rVB2	248915	777898	42.73%	8.019%

Sum of corrected areas: 9700408

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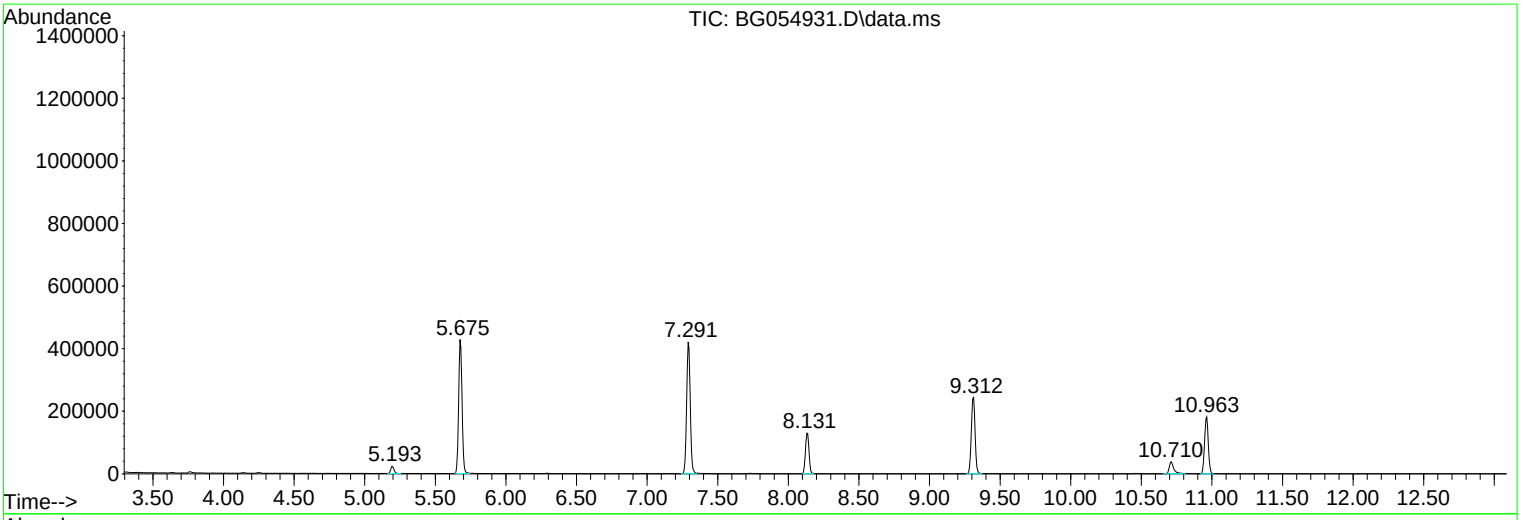
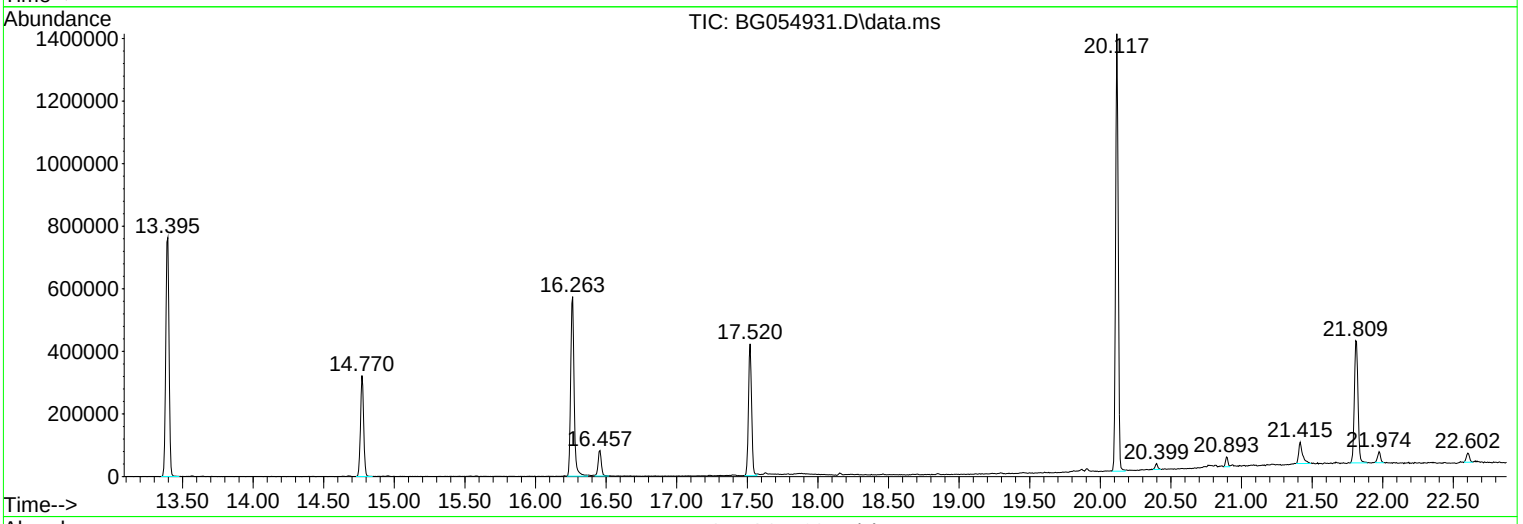
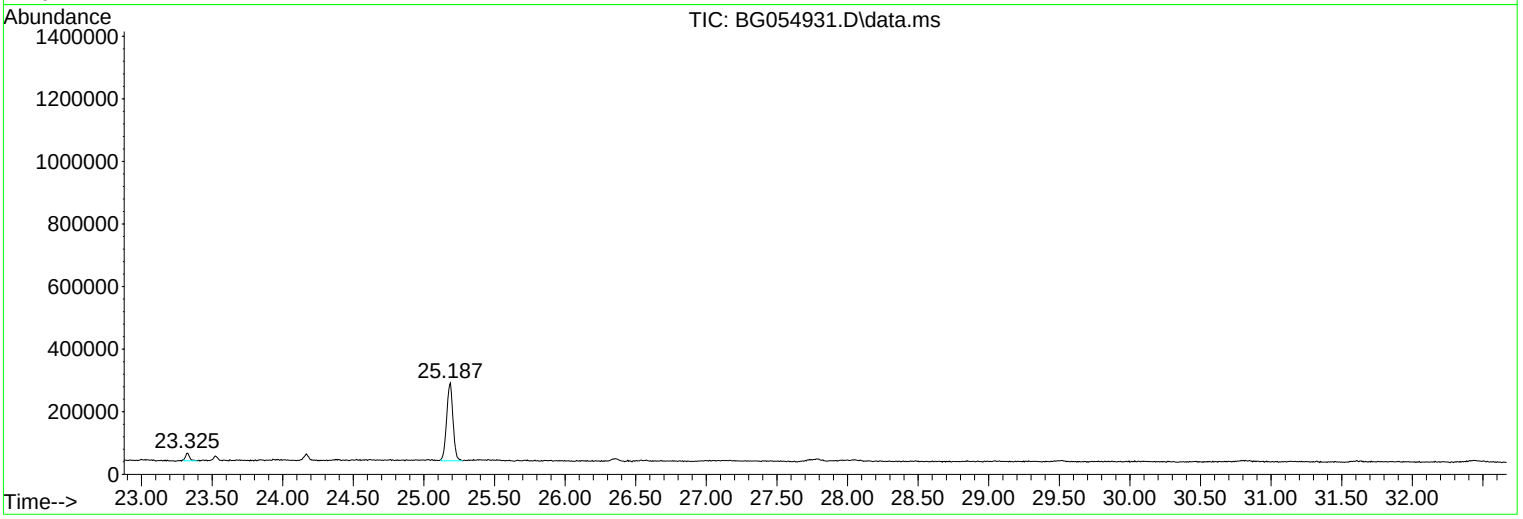
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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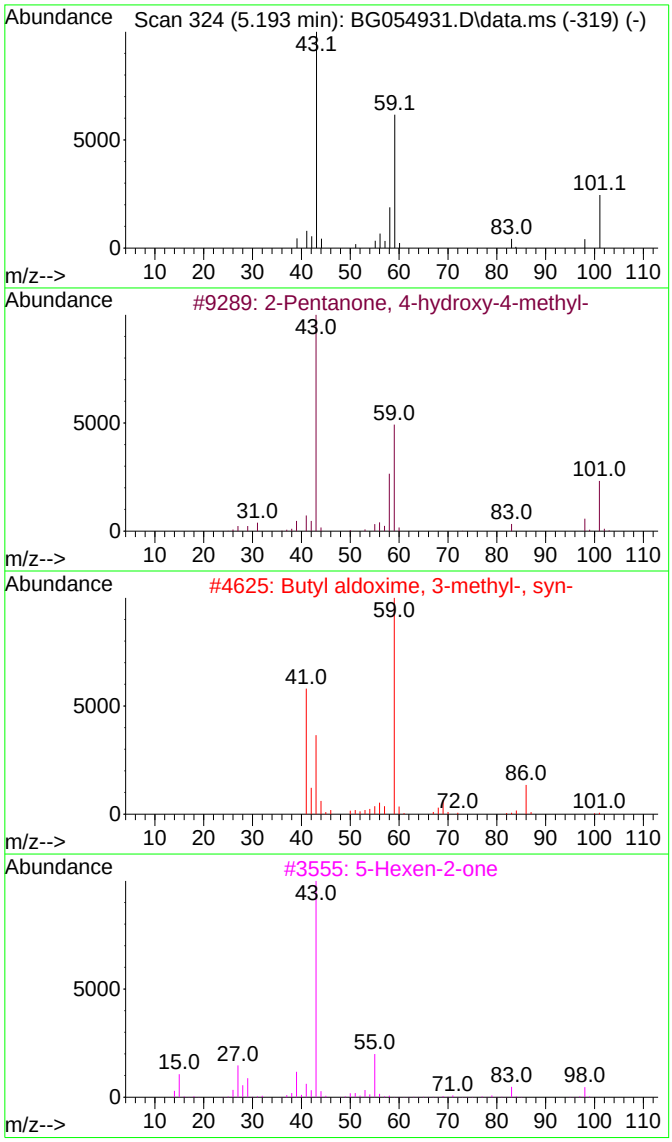
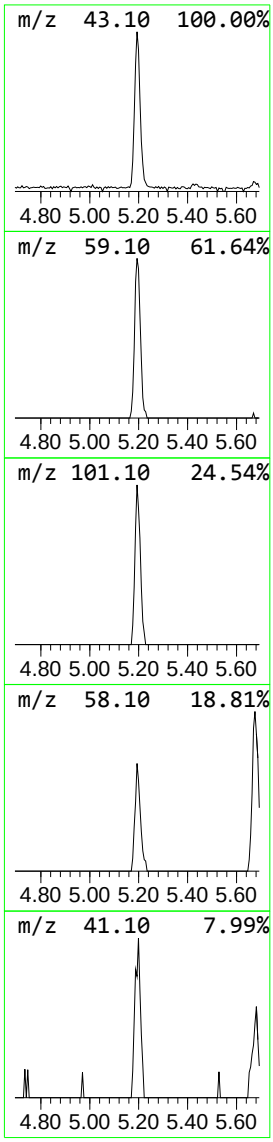
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.193	3.28 ng	37489	1,4-Dichlorobenzene-d4	8.137

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
3	5-Hexen-2-one	98	C6H10O	000109-49-9	12
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	1-Butanol, 3-methoxy-	104	C5H12O2	002517-43-3	9





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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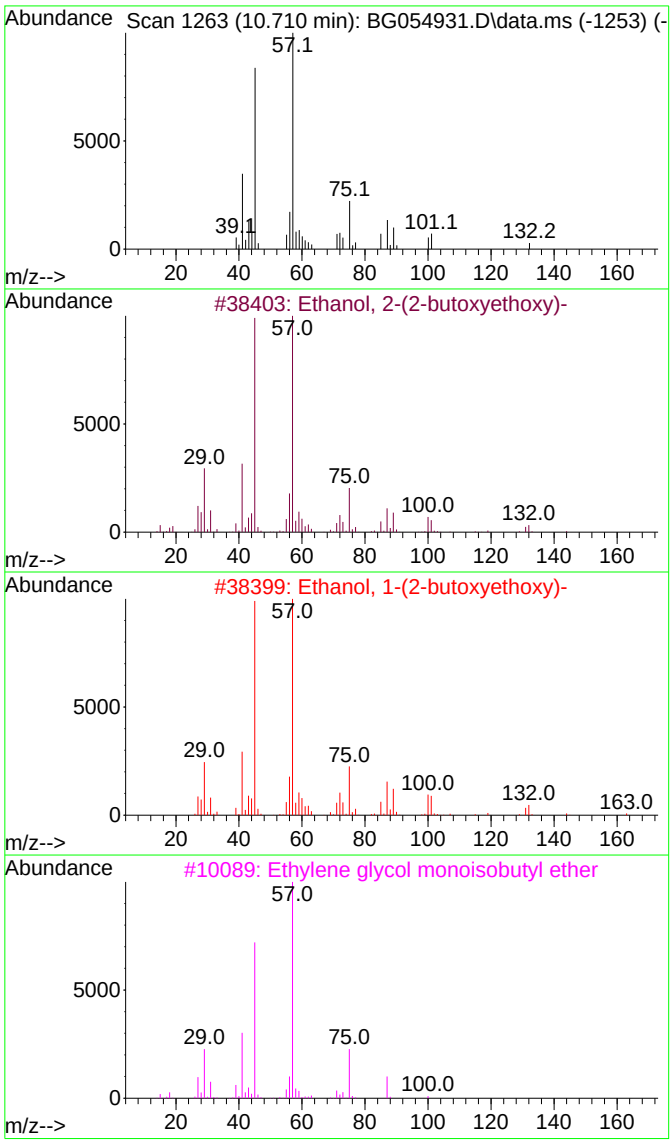
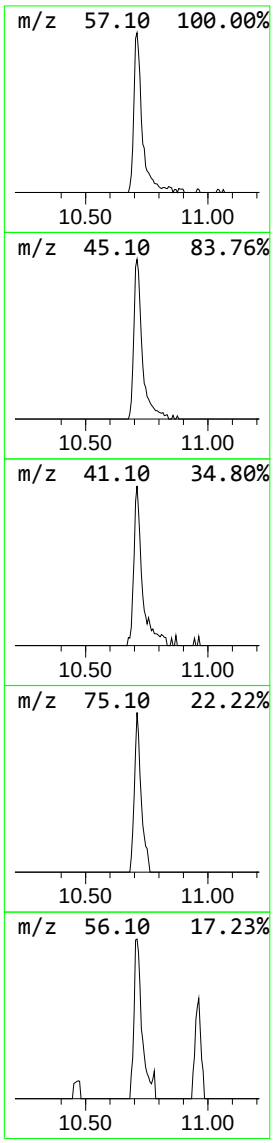
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.710	5.13 ng	84950	Naphthalene-d8	10.963

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	72
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
5	Butane, 1-(2-methoxyethoxy)-	132	C7H16O2	013343-98-1	45





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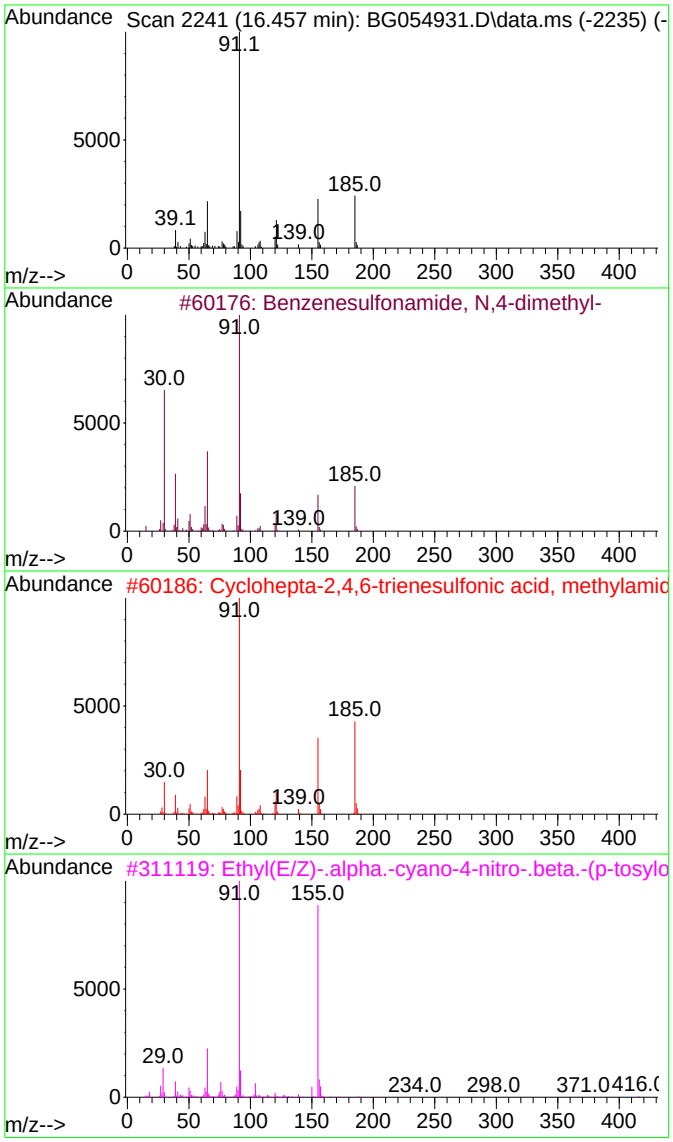
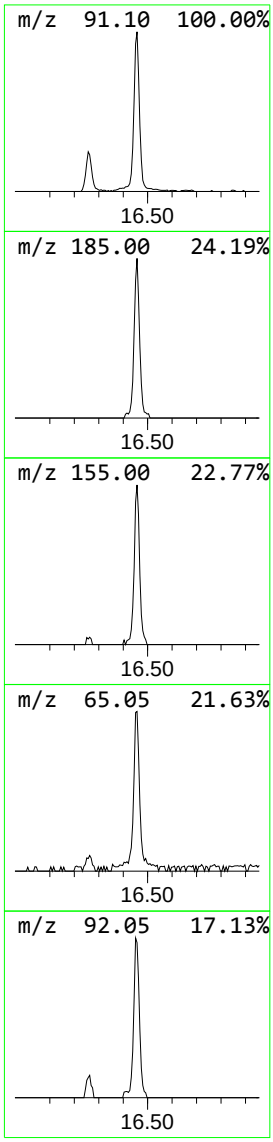
****
Peak Number 3 Benzenesulfonamide, N,4-dim... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.456	3.92 ng	127254	Phenanthrene-d10	17.520

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	95
2	Cyclohepta-2,4,6-trienesulfonic ...	185	C8H11NO2S	1000187-28-7	68
3	Ethyl(E/Z)-.alpha.-cyano-4-nitro...	416	C19H16N2O7S	1000287-26-8	53
4	4-Toluenesulfonylmethyl isocyanide	195	C9H9NO2S	036635-61-7	47
5	(O-p-Tosylisonitroso)malononitrile	249	C10H7N3O3S	020893-01-0	47





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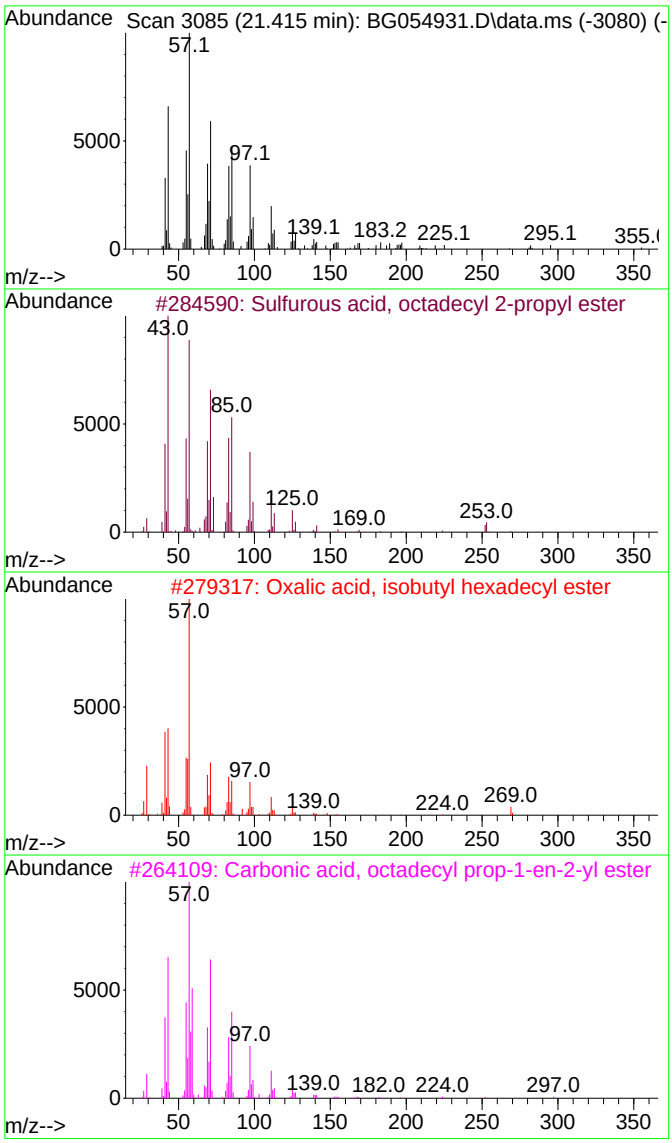
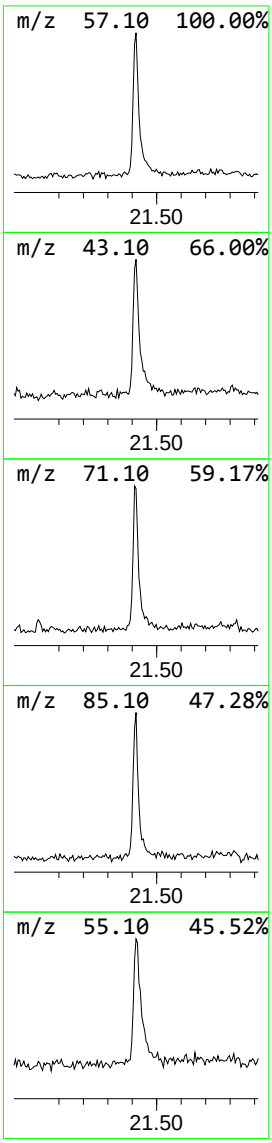
****
Peak Number 4 Sulfurous acid, octadecyl 2... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.415	3.70 ng	129783	Chrysene-d12	21.809

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	91
2	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	87
3	Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	83
4	Ethanol, 2-(octadecyloxy)-	314	C20H42O2	002136-72-3	83
5	Eicosyl isobutyl ether	354	C24H50O	1000406-33-0	74





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-...	5.193	3.3	ng	37489	1	8.137	228267	20.0
Ethanol, 2-(2-b...	10.710	5.1	ng	84950	2	10.963	330983	20.0
Benzenesulfonam...	16.456	3.9	ng	127254	4	17.520	649070	20.0
Sulfurous acid,...	21.415	3.7	ng	129783	5	21.809	700941	20.0