LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120522\
Data File : BG055892.D
Acq On : 5 Dec 2022 19:52
Operator : CG/JU
Sample : N5857-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP-SAMPLE-TANK-10-11-12-31-33

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-BG111622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055892.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.215	322	328	336	rBV	56937	87092	4.39%	0.817%
2	5.702	404	411	423	rVB	212385	343741	17.32%	3.224%
3	7.324	680	687	700	rBV	136755	238643	12.03%	2.238%
4	8.170	825	831	838	rBV	106099	169009	8.52%	1.585%
5	9.345	1024	1031	1041	rBV	345249	604777	30.48%	5.673%
6	11.002	1302	1313	1321	rBV	149150	269444	13.58%	2.527%
7	13.429	1718	1726	1732	rBV	981690	1528911	77.06%	14.341%
8	14.516	1907	1911	1914	rBV2	14822	20735	1.05%	0.194%
9	14.610	1921	1927	1931	rBV2	22767	34669	1.75%	0.325%
10	14.803	1953	1960	1967	rBV	280033	442082	22.28%	4.147%
11	14.921	1974	1980	1984	rBV5	14452	24545	1.24%	0.230%
12	15.749	2115	2121	2129	rVB7	24669	56368	2.84%	0.529%
13	16.290	2206	2213	2223	rBV	840357	1294463	65.24%	12.142%
14	16.648	2270	2274	2278	rVB4	11974	21102	1.06%	0.198%
15	17.541	2420	2426	2433	rBV	364143	547154	27.58%	5.132%
16	18.176	2530	2534	2539	rVB	24243	33721	1.70%	0.316%
17	18.405	2569	2573	2580	rBV2	48958	78501	3.96%	0.736%
18	18.481	2580	2586	2591	rVB	1546634	1984078	100.00%	18.610%
19	19.662	2783	2787	2798	rBV4	28816	57791	2.91%	0.542%
20	20.132	2861	2867	2875	rVB	1096688	1424227	71.78%	13.359%
21	21.437	3084	3089	3103	rVB4	30809	90352	4.55%	0.847%
22	21.825	3149	3155	3162	rVB2	353568	590032	29.74%	5.534%
23	23.000	3350	3355	3361	rVB2	48882	85563	4.31%	0.803%
24	25.179	3715	3726	3739	rVB2	205684	634224	31.97%	5.949%

Sum of corrected areas: 10661224

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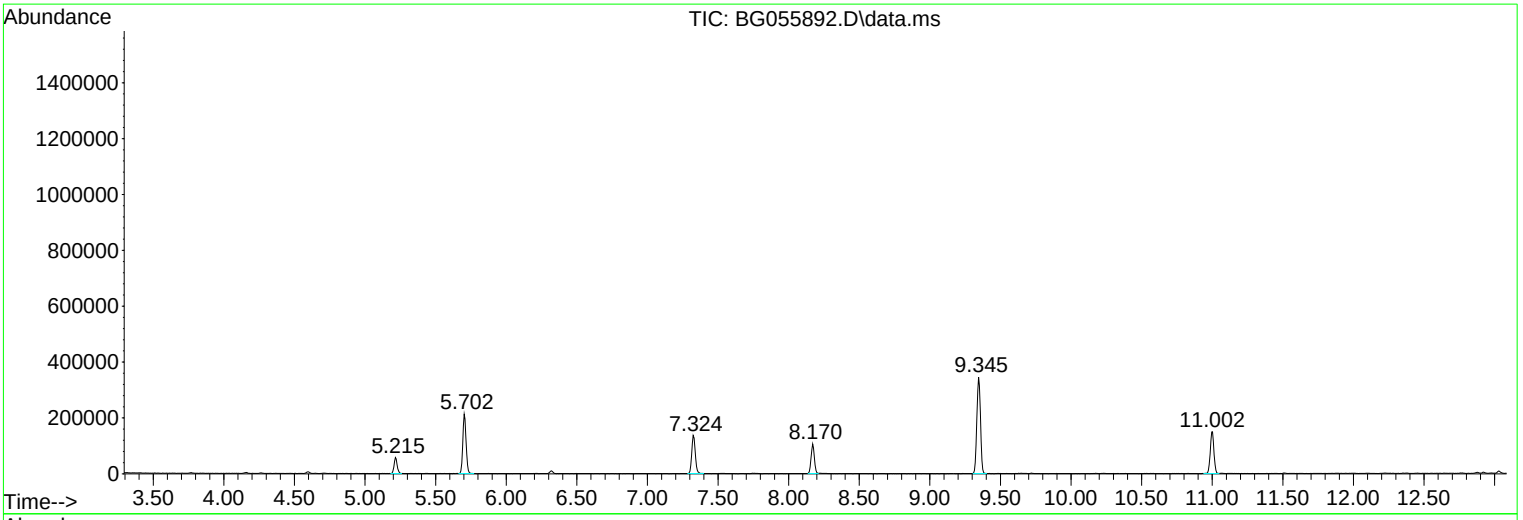
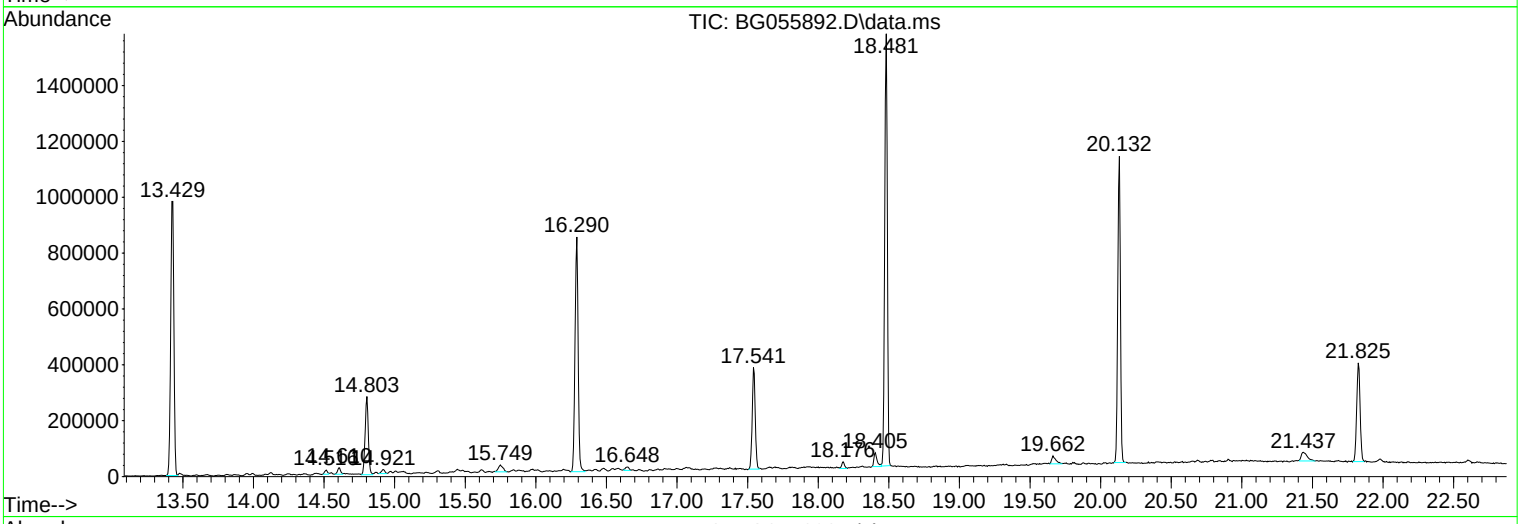
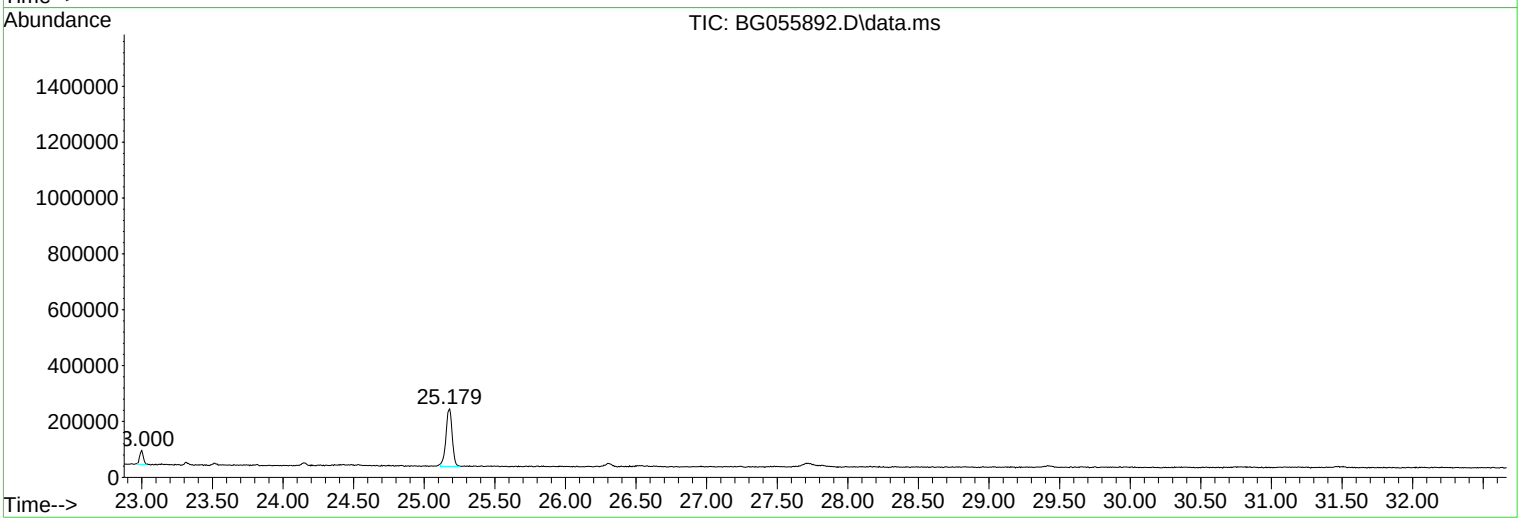
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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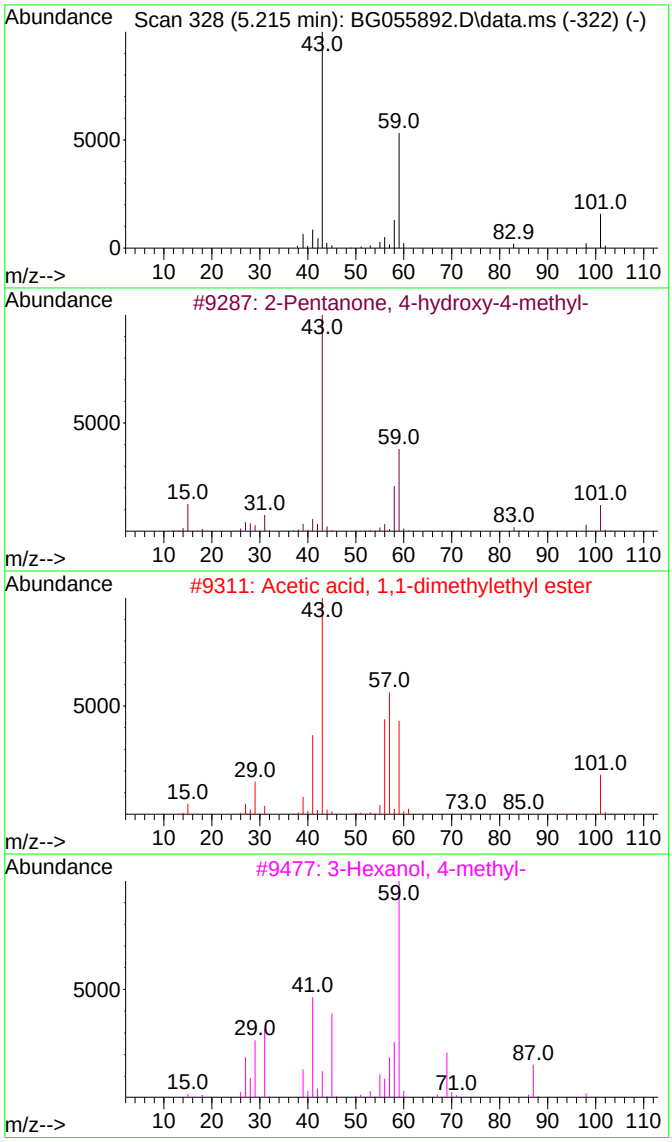
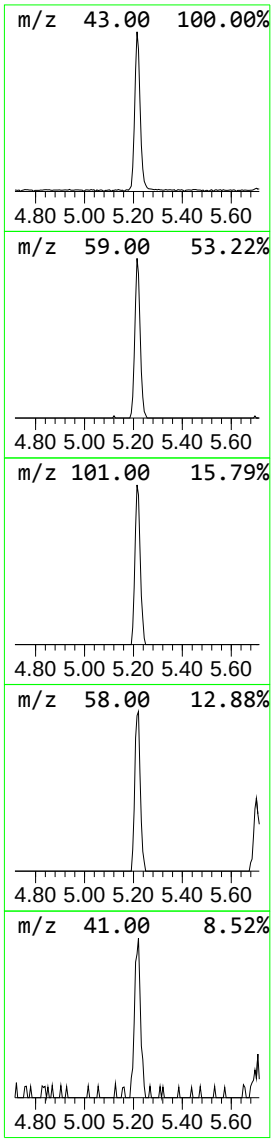
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.215	10.31 ng	87092	1,4-Dichlorobenzene-d4	8.170

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





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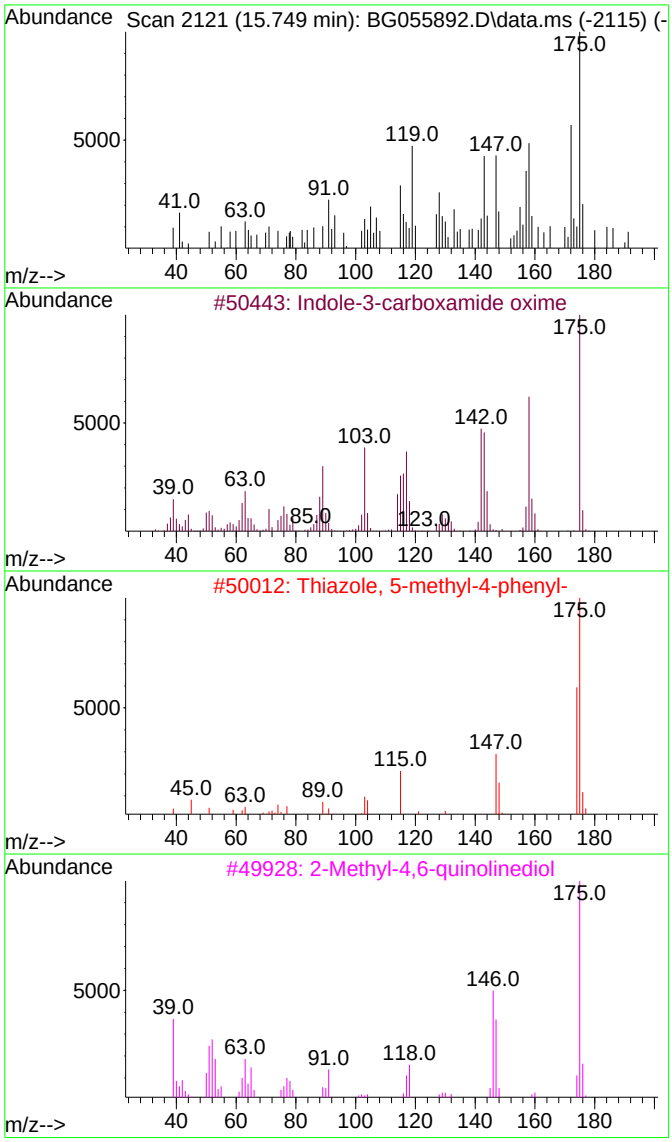
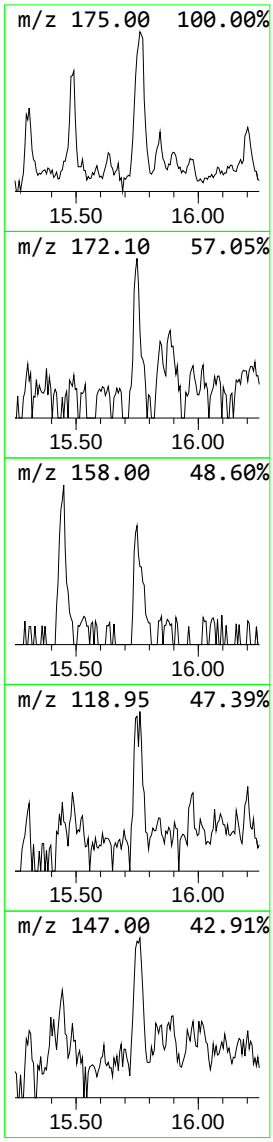
****

Peak Number 2 Indole-3-carboxamide oxime Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.749	2.55 ng	56368	Acenaphthene-d10	14.803

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indole-3-carboxamide oxime	175	C9H9N3O	095649-37-9	50
2	Thiazole, 5-methyl-4-phenyl-	175	C10H9NS	001826-18-2	30
3	2-Methyl-4,6-quinolinediol	175	C10H9NO2	034982-04-2	27
4	3-Aminocoumarin, N-methyl-	175	C10H9NO2	1000451-94-3	22
5	1H,2H,3H,4H-Pyrazino[1,2-a]indole	172	C11H12N2	041838-39-5	15





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Instrument :
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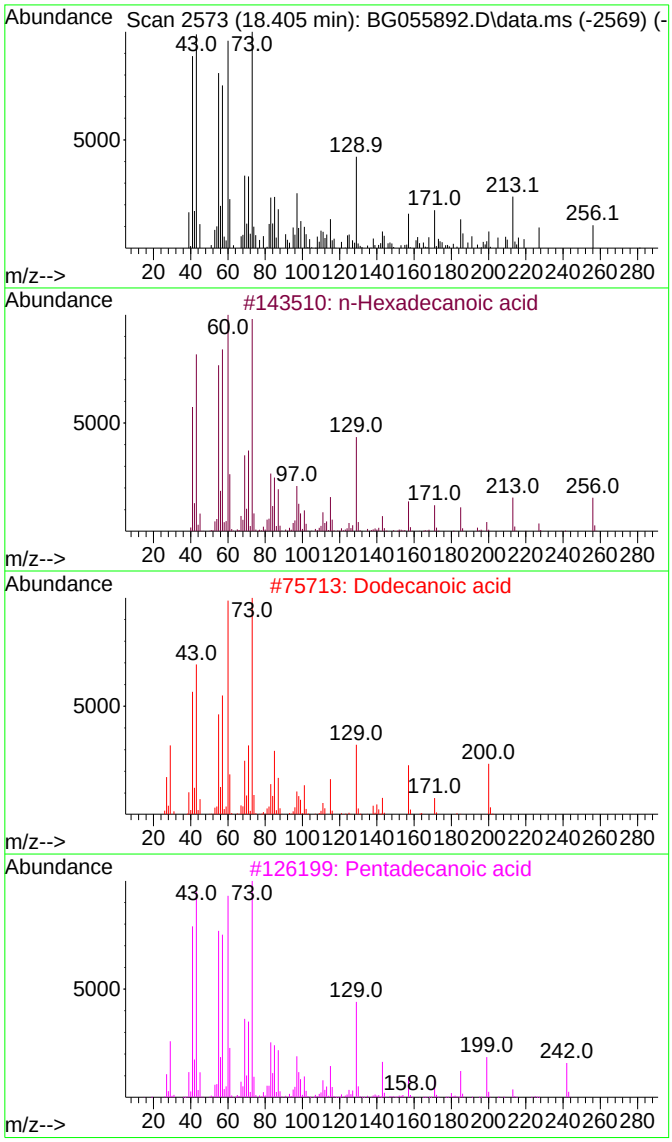
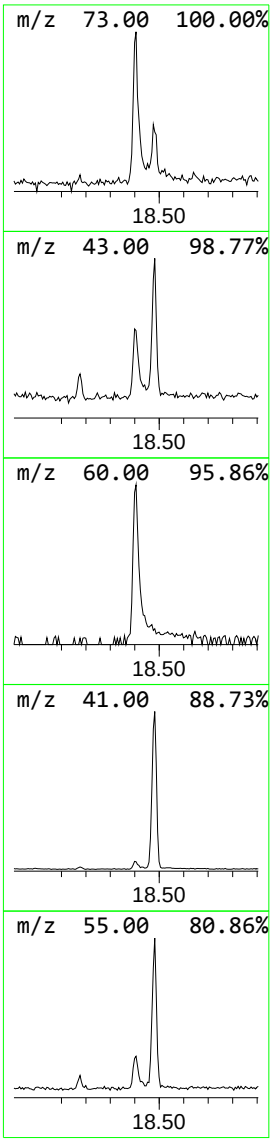
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.405	2.87 ng	78501	Phenanthrene-d10	17.541

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Dodecanoic acid	200	C12H24O2	000143-07-7	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5	Undecanoic acid	186	C11H22O2	000112-37-8	64





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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
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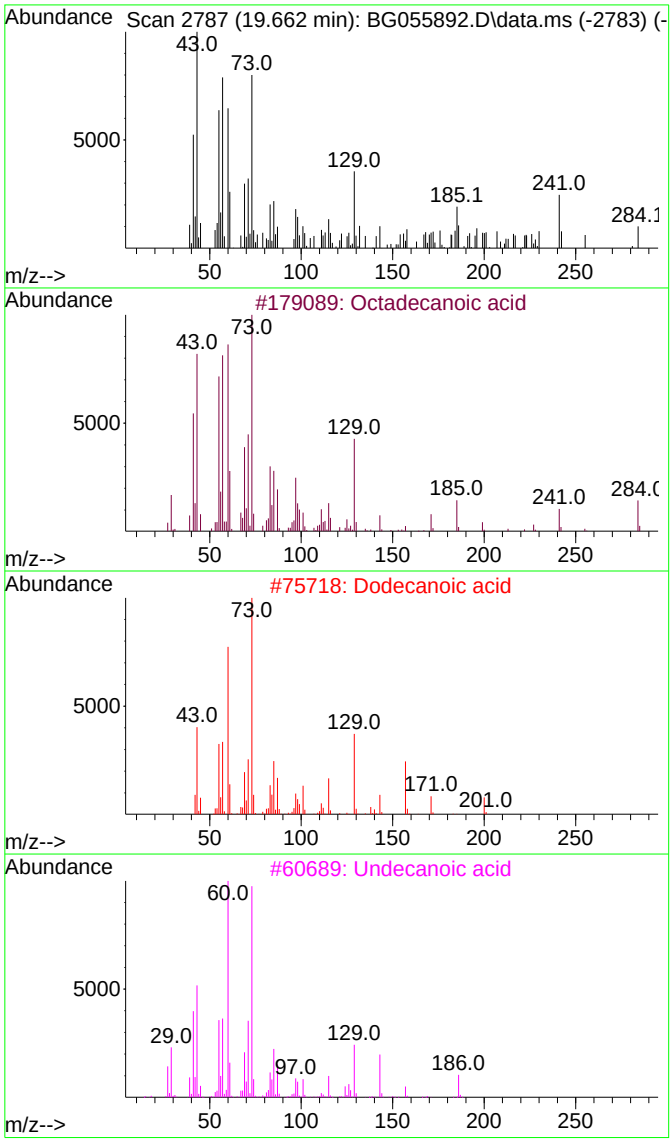
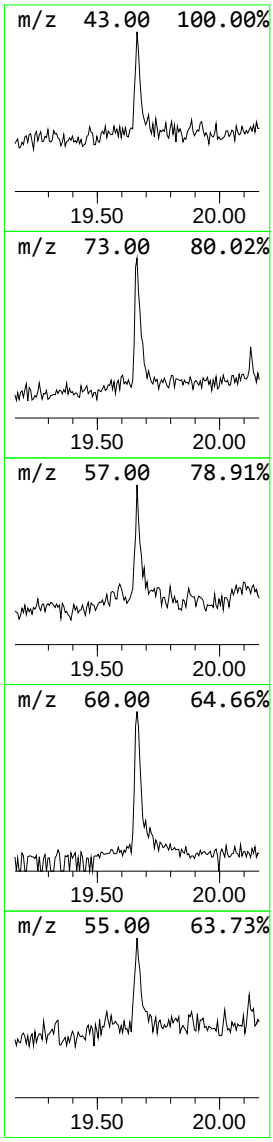
****

Peak Number 4 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.662	2.11 ng	57791	Phenanthrene-d10	17.541

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	60
2	Dodecanoic acid	200	C12H24O2	000143-07-7	55
3	Undecanoic acid	186	C11H22O2	000112-37-8	55
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	49
5	n-Decanoic acid	172	C10H20O2	000334-48-5	38





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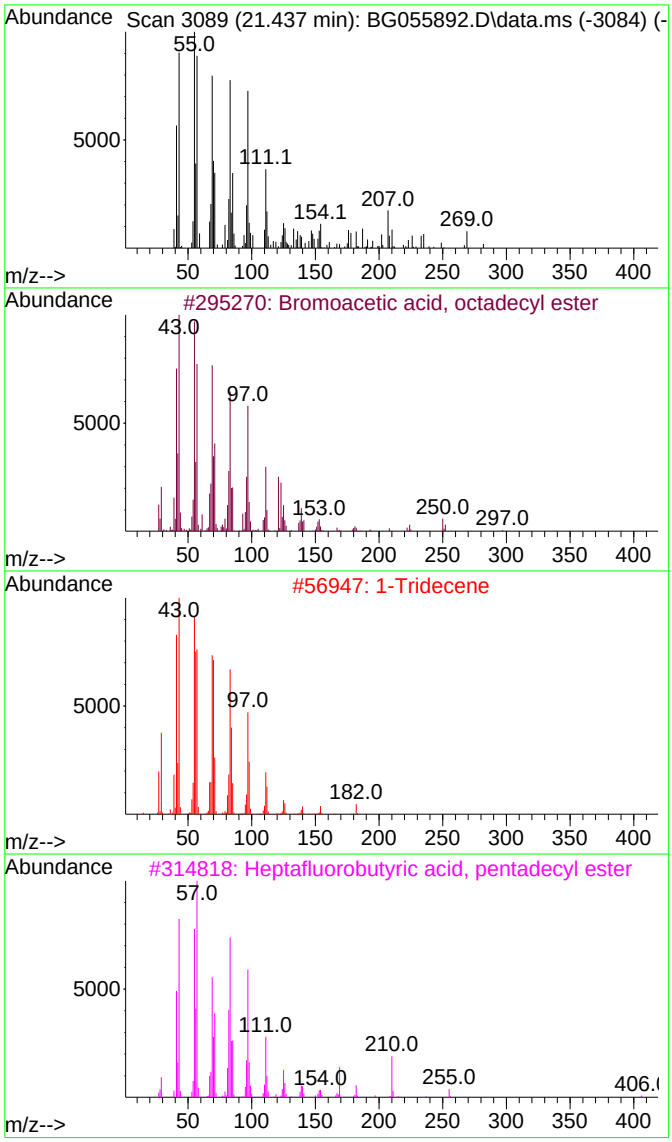
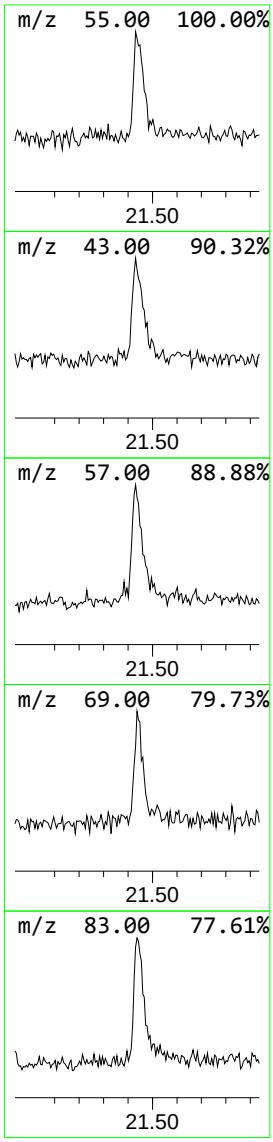
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Bromoacetic acid, octadecyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.437	3.06 ng	90352	Chrysene-d12	21.825

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	68
2	1-Tridecene	182	C13H26	002437-56-1	64
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	64
4	1-Pentadecene	210	C15H30	013360-61-7	58
5	Cyclopentane, 1-pentyl-2-propyl-	182	C13H26	062199-51-3	58





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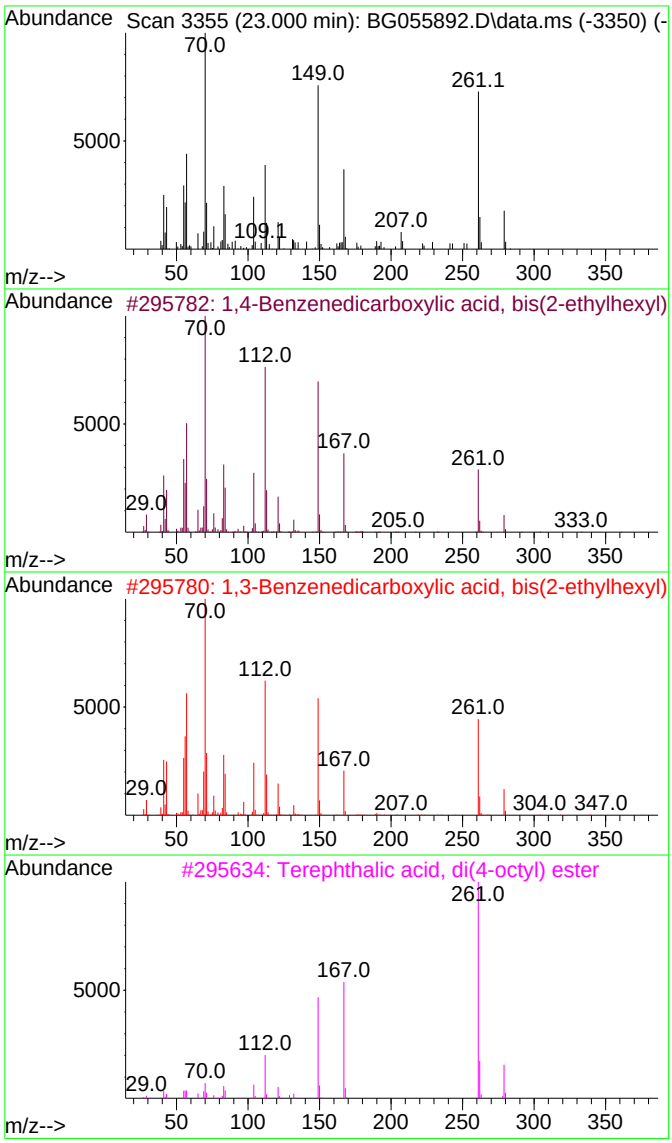
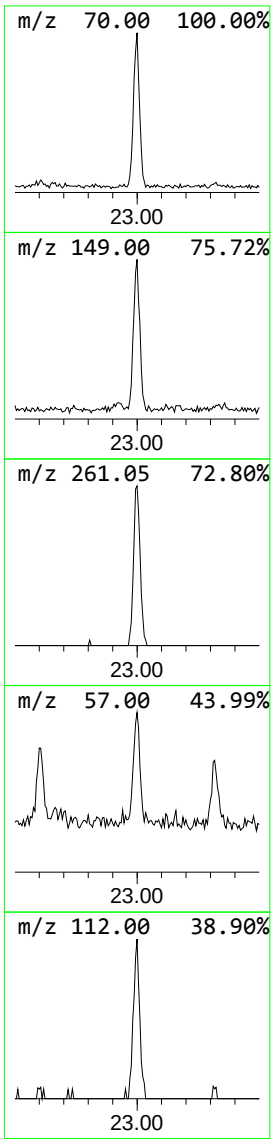
****
Peak Number 6 1,4-Benzenedicarboxylic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.000	2.90 ng	85563	Chrysene-d12	21.825

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	52
2	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	43
3	Terephthalic acid, di(4-octyl) e...	390	C24H38O4	1000323-74-2	43
4	Terephthalic acid, dodec-2-enyl ...	444	C28H44O4	1000356-30-9	38
5	Phthalic acid, but-3-yn-2-yl 3,5...	330	C18H12F2O4	1000315-75-6	35





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-...	5.215	10.3	ng	87092	1	8.170	169009	20.0
Indole-3-carbox...	15.749	2.5	ng	56368	3	14.803	442082	20.0
n-Hexadecanoic ...	18.405	2.9	ng	78501	4	17.541	547154	20.0
Octadecanoic acid	19.662	2.1	ng	57791	4	17.541	547154	20.0
Bromoacetic aci...	21.437	3.1	ng	90352	5	21.825	590032	20.0
1,4-Benzenedica...	23.000	2.9	ng	85563	5	21.825	590032	20.0