LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051052.D
Acq On : 15 Nov 2021 22:08
Operator : CG/JU
Sample : M4681-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP-2

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: BG051052.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.291	298	307	314	rBV	26487	44077	1.48%	0.273%
2	5.761	378	387	396	rBV	988415	1609237	53.99%	9.965%
3	7.371	653	661	674	rBV	954634	1744133	58.51%	10.801%
4	8.223	799	806	813	rBV	150269	260326	8.73%	1.612%
5	9.398	997	1006	1019	rBV	588111	1093651	36.69%	6.773%
6	10.797	1236	1244	1265	rBV	254690	474101	15.91%	2.936%
7	11.049	1280	1287	1295	rVB	205807	379715	12.74%	2.351%
8	13.470	1691	1699	1708	rBV	1458764	2309595	77.49%	14.302%
9	13.717	1733	1741	1749	rVB	45136	73470	2.46%	0.455%
10	14.851	1927	1934	1943	rVB	350623	555365	18.63%	3.439%
11	15.785	2088	2093	2101	rVB	30029	46932	1.57%	0.291%
12	16.267	2169	2175	2180	rBV6	16476	34577	1.16%	0.214%
13	16.337	2180	2187	2196	rVB	1159406	1785668	59.91%	11.058%
14	17.594	2395	2401	2408	rBV	432632	666977	22.38%	4.130%
15	17.706	2415	2420	2427	rBV3	37354	55074	1.85%	0.341%
16	18.223	2503	2508	2518	rVB	43498	57151	1.92%	0.354%
17	18.446	2541	2546	2553	rBV	129175	187528	6.29%	1.161%
18	19.386	2702	2706	2711	rVB	97055	120711	4.05%	0.748%
19	19.516	2723	2728	2732	rBV2	26128	34152	1.15%	0.211%
20	19.710	2756	2761	2768	rBV	55993	86989	2.92%	0.539%
21	20.186	2835	2842	2849	rBV	2216584	2980679	100.00%	18.458%
22	20.444	2881	2886	2893	rBV5	29001	68313	2.29%	0.423%
23	20.802	2943	2947	2951	rBV	34628	42559	1.43%	0.264%
24	21.490	3059	3064	3074	rBV	124998	239232	8.03%	1.481%
25	21.895	3127	3133	3141	rVB2	349314	604067	20.27%	3.741%
26	25.303	3704	3713	3724	rVB2	189892	594099	19.93%	3.679%

Sum of corrected areas: 16148378

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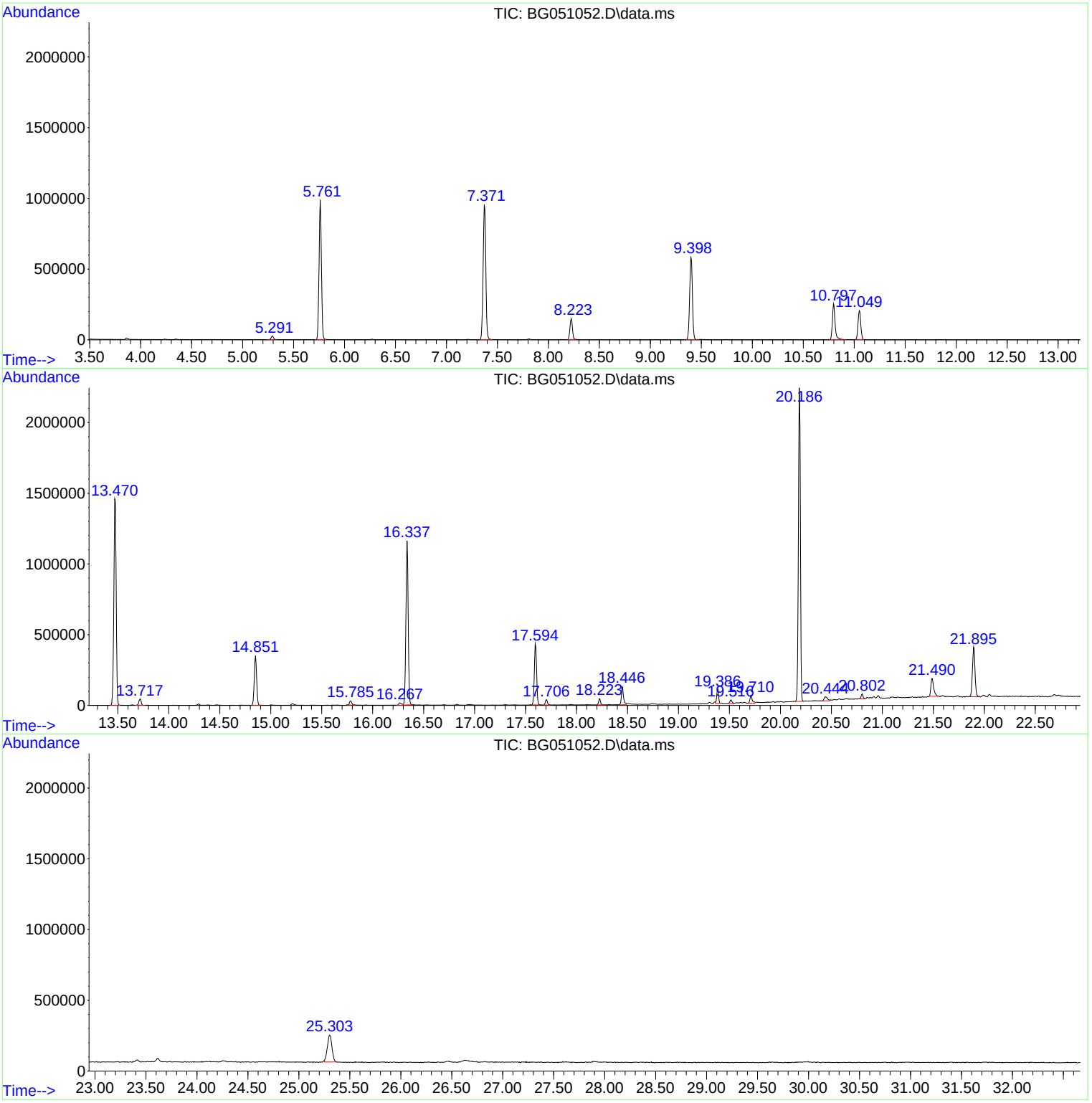
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BG051052.D
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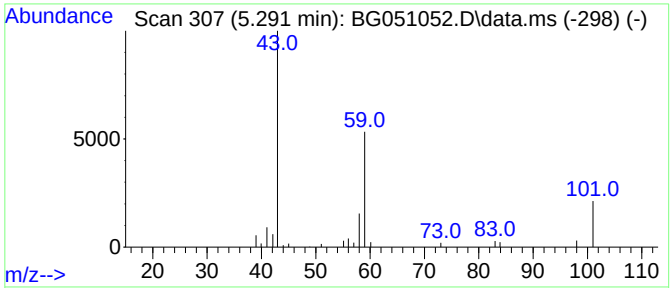
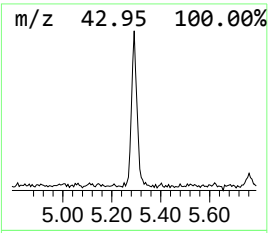
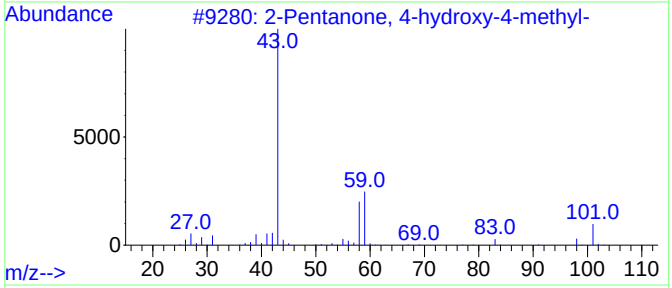
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

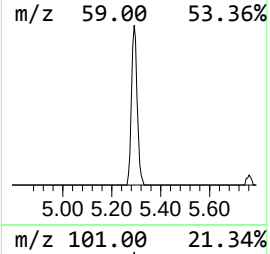
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.291	3.39 ng	44077	1,4-Dichlorobenzene-d4	8.223

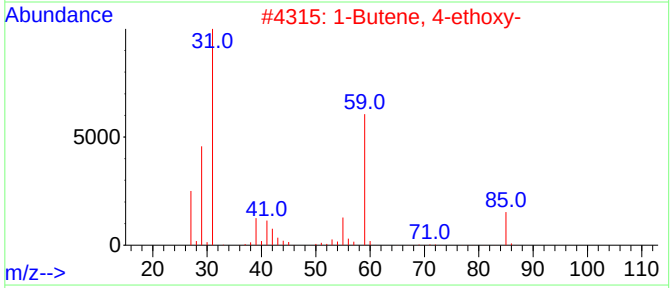
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	1-Butene, 4-ethoxy-	100	C6H12O	044611-46-3	17
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	4-Pentene-2-ol, 2-methyl	100	C6H12O	000624-97-5	9
5	DL-Lactamide, N,O-dimethyl-	117	C5H11NO2	1000452-56-3	9

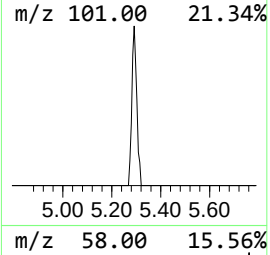


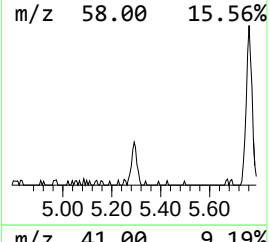


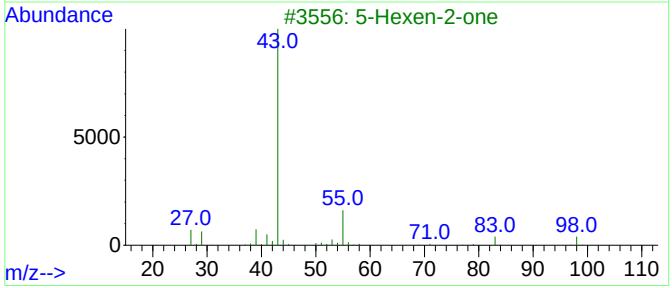


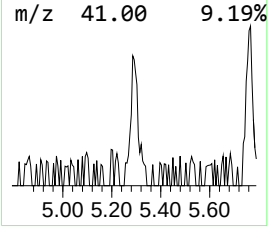












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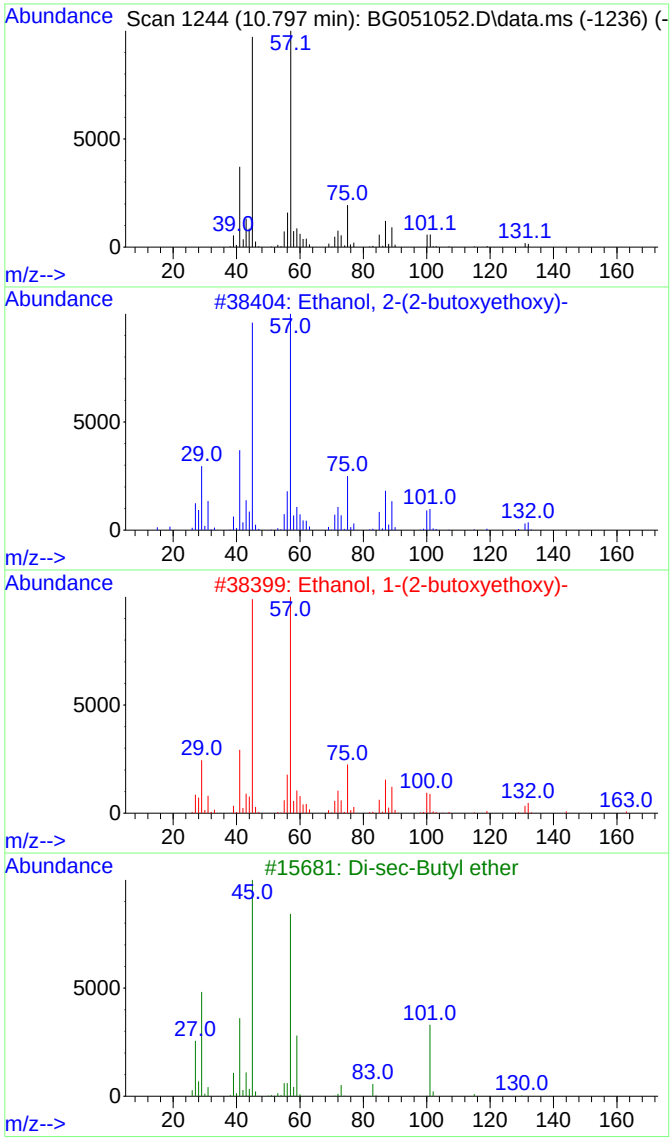
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

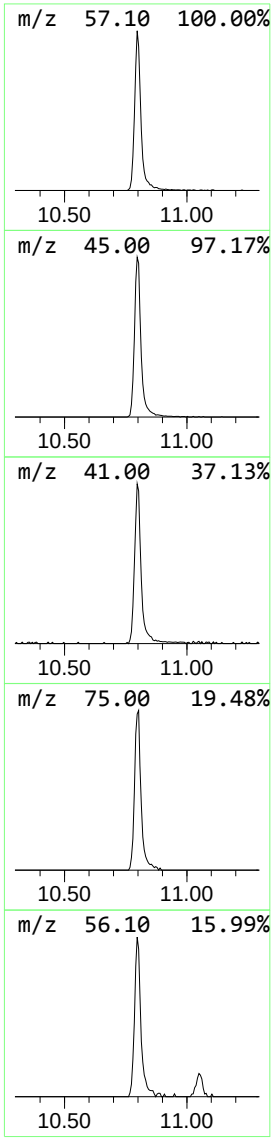
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.797	24.97 ng	474101	Naphthalene-d8	11.049

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	Di-sec-Butyl ether	130	C8H18O	006863-58-7	50
4	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50
5	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50





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TIC Library : C:\Database\NIST20.L
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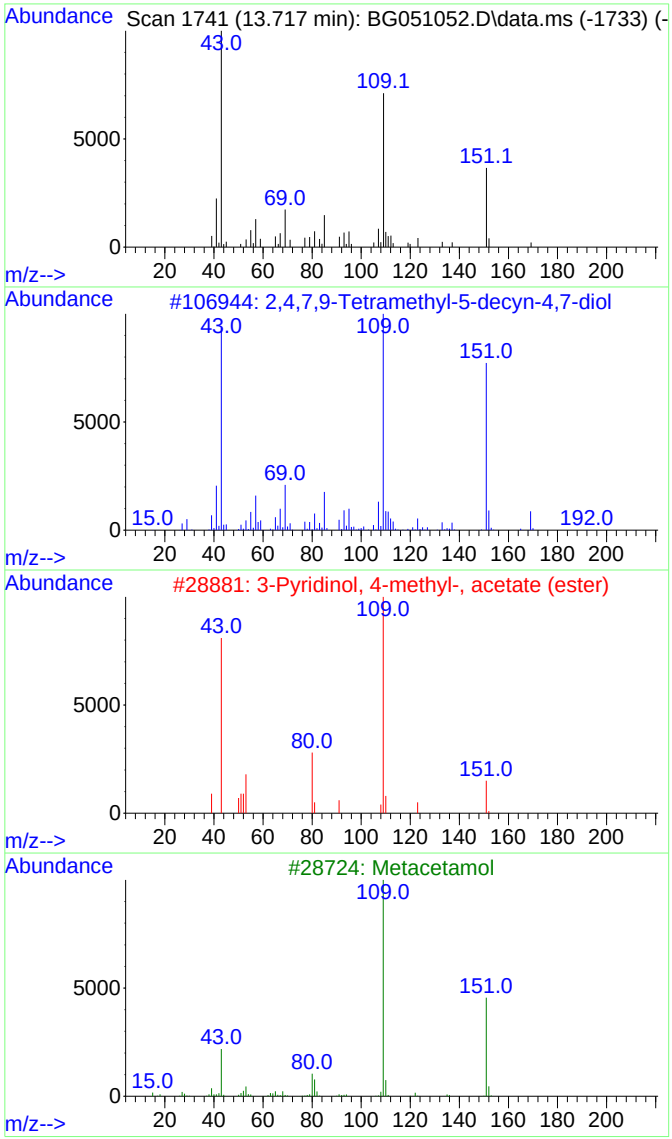
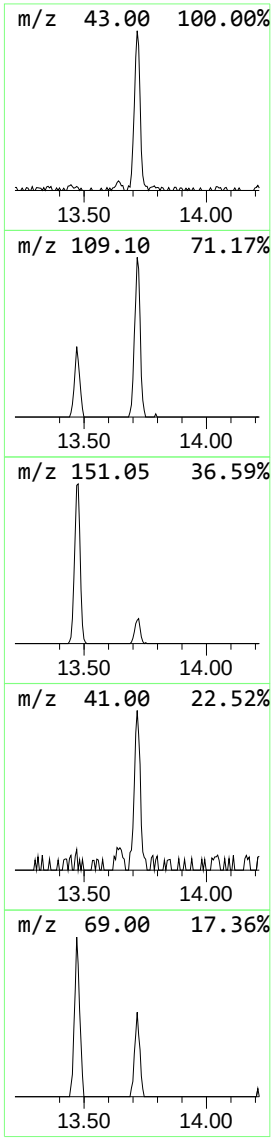
****
Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.717	2.65 ng	73470	Acenaphthene-d10	14.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	90
2	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	53
3	Metacetamol	151	C8H9NO2	000621-42-1	52
4	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	50
5	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	50





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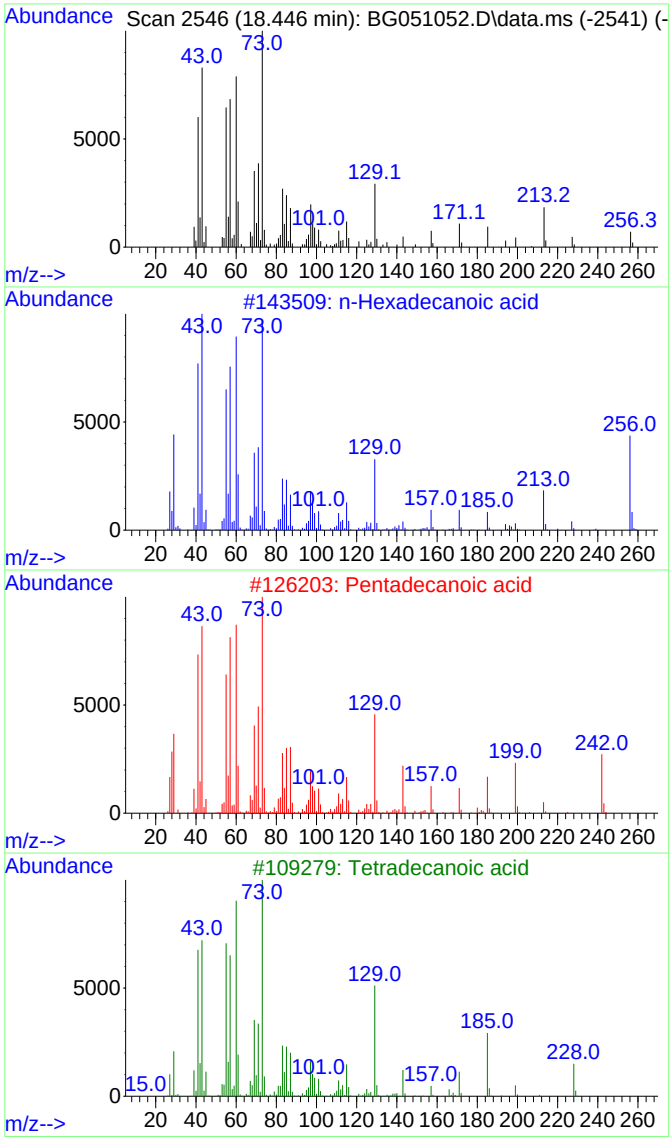
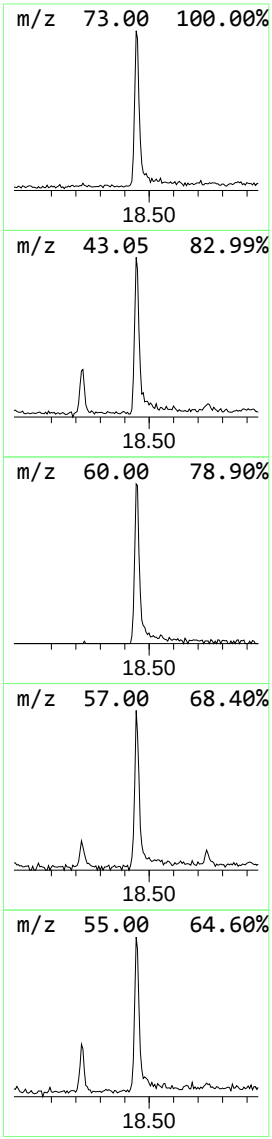
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.446	5.62 ng	187528	Phenanthrene-d10	17.594

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	Nonanoic acid	158	C9H18O2	000112-05-0	30





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Instrument :
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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
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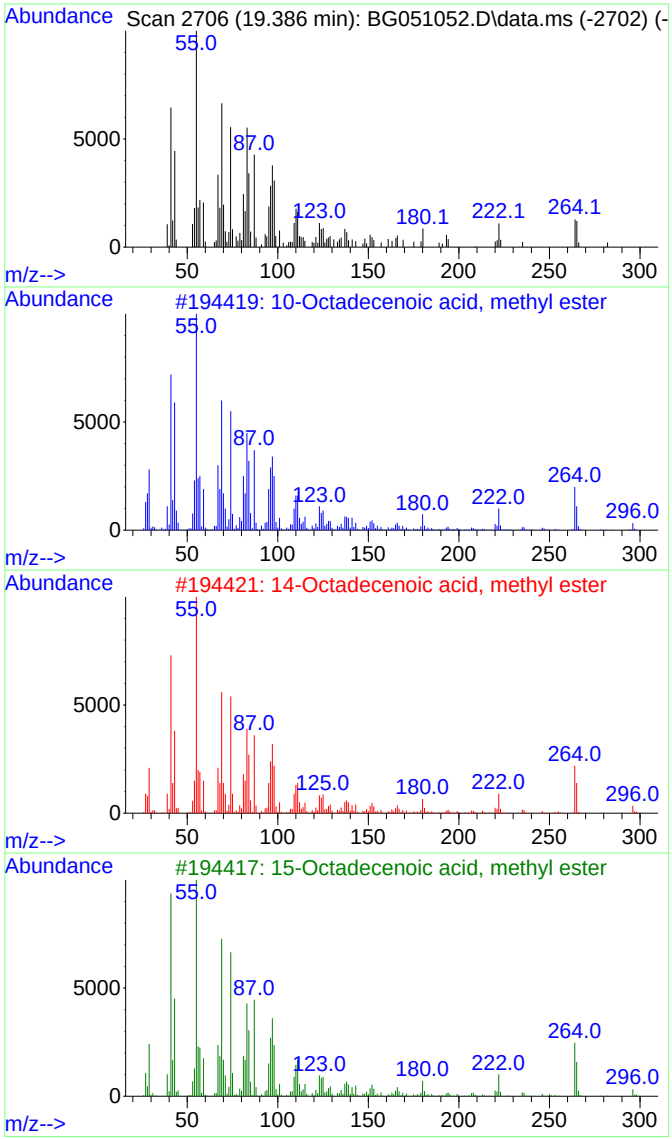
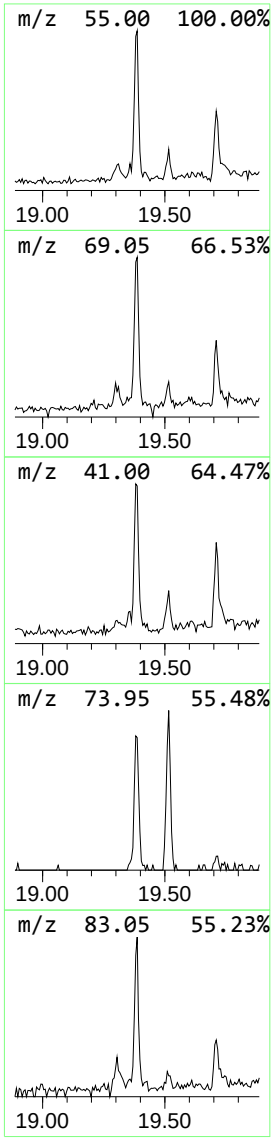
****
Peak Number 5 10-Octadecenoic acid, methy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.387	3.62 ng	120711	Phenanthrene-d10	17.594

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	94
2	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	91
3	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	90
4	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	87
5	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	87





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TIC Library : C:\Database\NIST20.L
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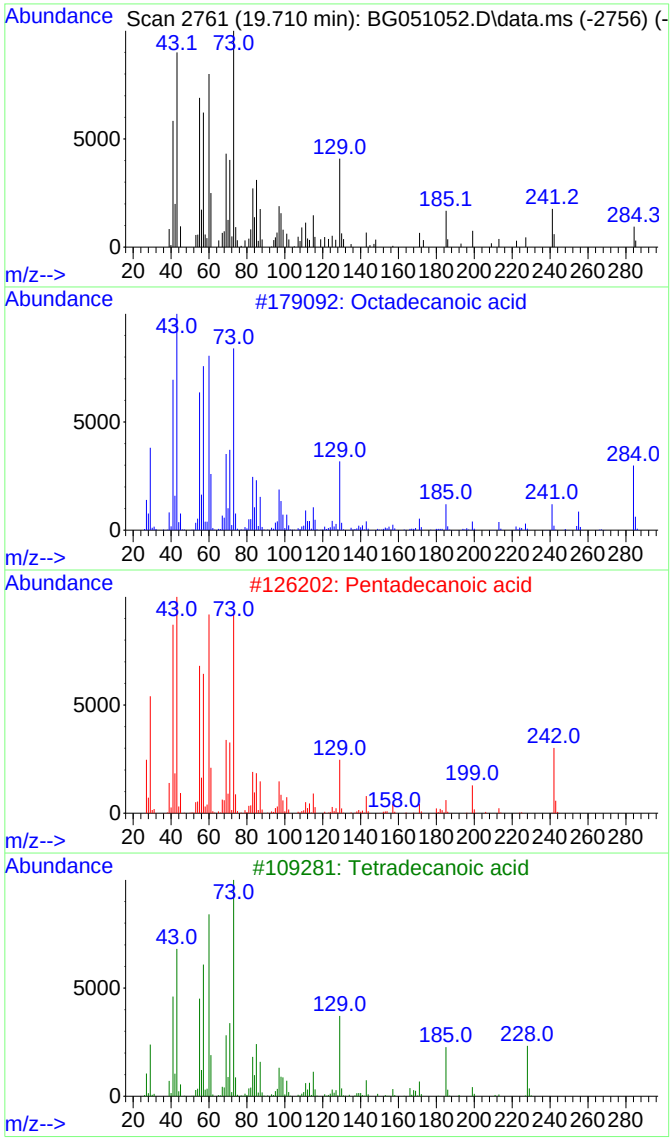
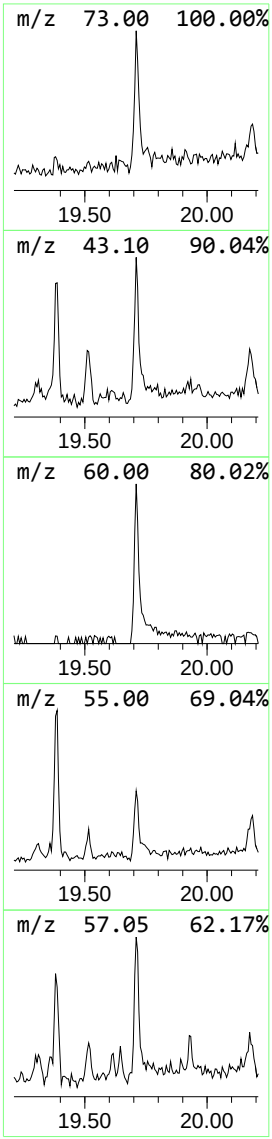
****

Peak Number 6 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.710	2.61 ng	86989	Phenanthrene-d10	17.594

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
5	Xylose	150	C5H10O5	000058-86-6	27





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TIC Library : C:\Database\NIST20.L
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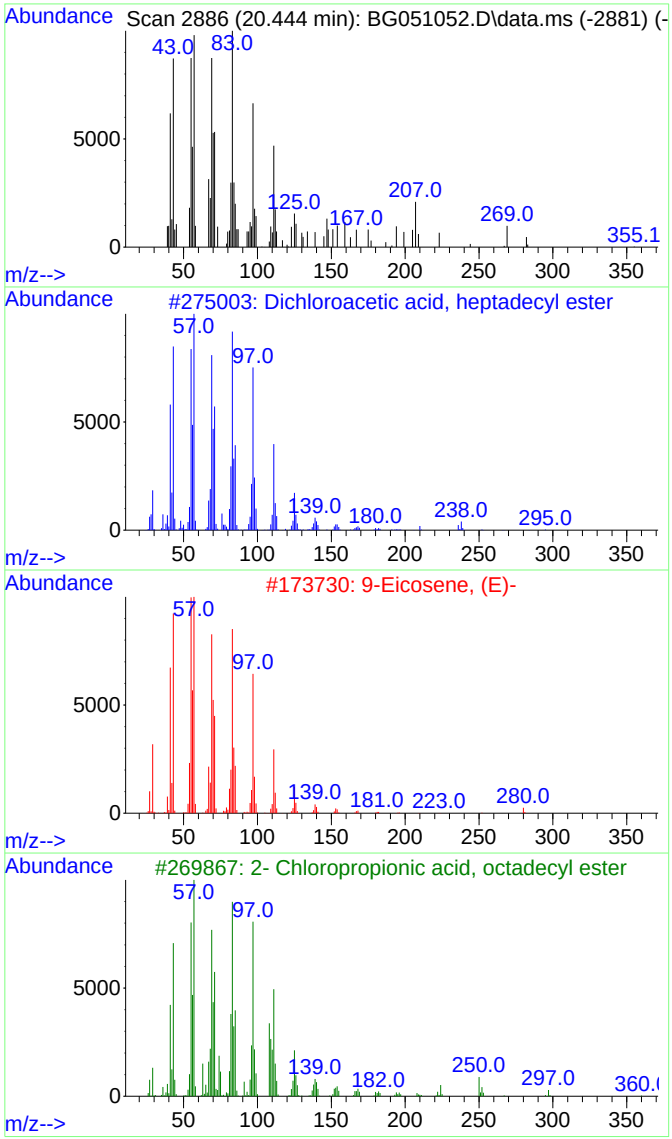
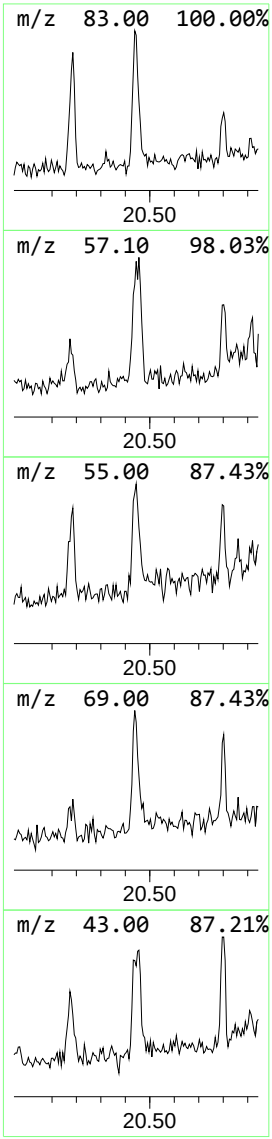
****
Peak Number 7 Dichloroacetic acid, heptad... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.444	2.26 ng	68313	Chrysene-d12	21.895

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	87
2	9-Eicosene, (E)-	280	C20H40	074685-29-3	87
3	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	83
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	83
5	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	74





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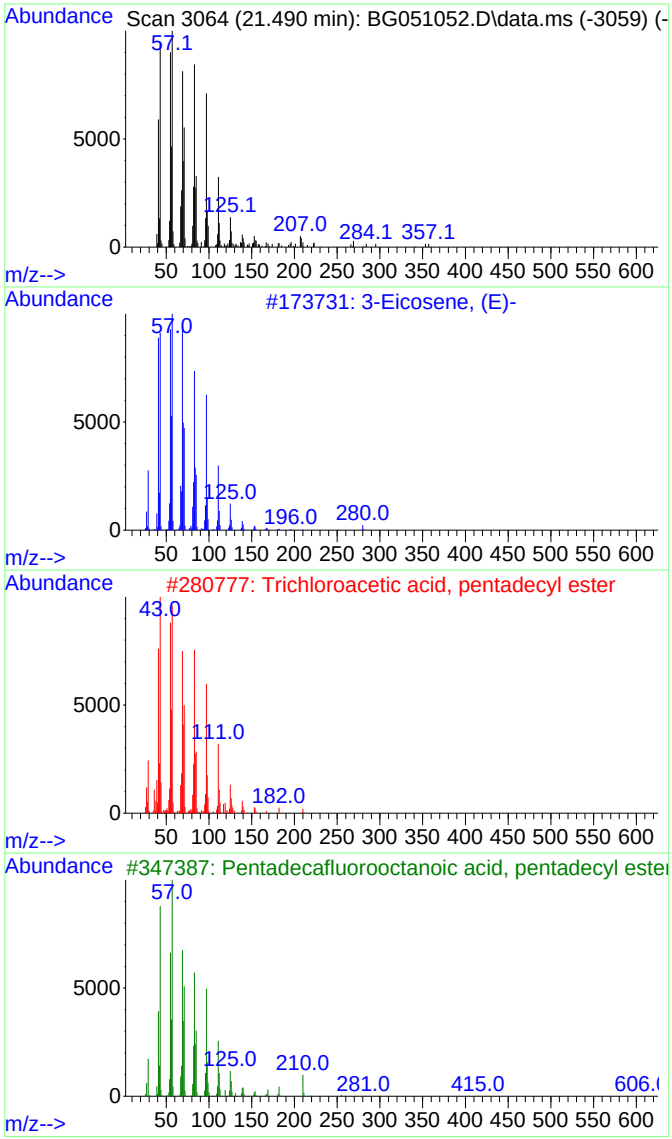
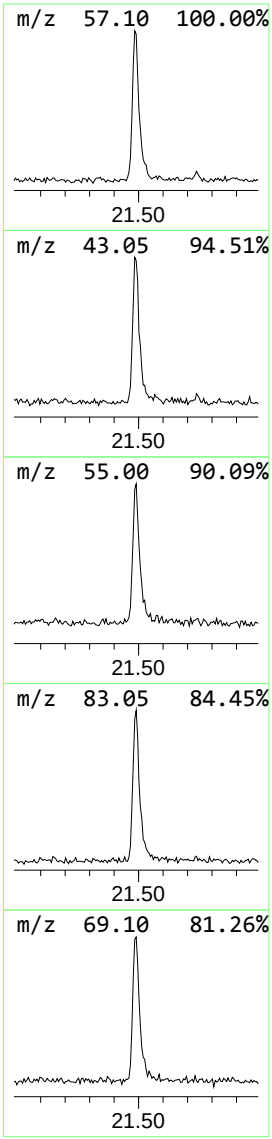
****

Peak Number 8 3-Eicosene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.490	7.92 ng	239232	Chrysene-d12	21.895

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	94
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
3	Pentadecafluorooctanoic acid, pe...	624	C23H31F15O2	1000406-04-5	94
4	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	94
5	1-Hexacosene	364	C26H52	018835-33-1	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
Data File : BG051052.D
Acq On : 15 Nov 2021 22:08
Operator : CG/JU
Sample : M4681-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP-2

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	5.291	3.4	ng	44077	1	8.223	260326	20.0
Ethanol, 2-(2-b...	10.797	25.0	ng	474101	2	11.049	379715	20.0
2,4,7,9-Tetrame...	13.717	2.6	ng	73470	3	14.851	555365	20.0
n-Hexadecanoic ...	18.446	5.6	ng	187528	4	17.594	666977	20.0
10-Octadecenoic...	19.387	3.6	ng	120711	4	17.594	666977	20.0
Octadecanoic acid	19.710	2.6	ng	86989	4	17.594	666977	20.0
Dichloroacetic ...	20.444	2.3	ng	68313	5	21.895	604067	20.0
3-Eicosene, (E)-	21.490	7.9	ng	239232	5	21.895	604067	20.0