LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041222\
Data File : BG053126.D
Acq On : 12 Apr 2022 19:15
Operator : CG/JU
Sample : N2334-10
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-25

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-BG040822.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053126.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	306	311	318	rBV	22337	37286	1.07%	0.234%
2	5.684	384	391	404	rVB	359029	593422	17.06%	3.723%
3	7.276	655	662	674	rVB	248836	436677	12.55%	2.740%
4	8.122	799	806	812	rBV	126723	217490	6.25%	1.364%
5	9.280	995	1003	1012	rBV	498892	922275	26.51%	5.786%
6	9.432	1023	1029	1044	rBV3	48957	115688	3.33%	0.726%
7	10.214	1155	1162	1169	rBV	85880	147046	4.23%	0.923%
8	10.930	1277	1284	1292	rBV	169457	307890	8.85%	1.932%
9	13.368	1691	1699	1706	rBV	1356459	2122989	61.02%	13.319%
10	14.150	1825	1832	1840	rBV3	28213	62986	1.81%	0.395%
11	14.631	1892	1914	1927	rBV	890939	3478985	100.00%	21.826%
12	14.743	1927	1933	1943	rVB	270958	461790	13.27%	2.897%
13	16.229	2177	2186	2195	rBV	1166883	1832382	52.67%	11.496%
14	17.486	2393	2400	2409	rVB	362462	560700	16.12%	3.518%
15	20.089	2836	2843	2851	rBV	2521713	3291572	94.61%	20.650%
16	21.393	3061	3065	3069	rBV3	27330	39280	1.13%	0.246%
17	21.763	3122	3128	3137	rVB2	361858	621922	17.88%	3.902%
18	22.955	3326	3331	3337	rBV4	30223	51342	1.48%	0.322%
19	25.070	3680	3691	3706	rVB2	218569	637958	18.34%	4.002%

Sum of corrected areas: 15939680

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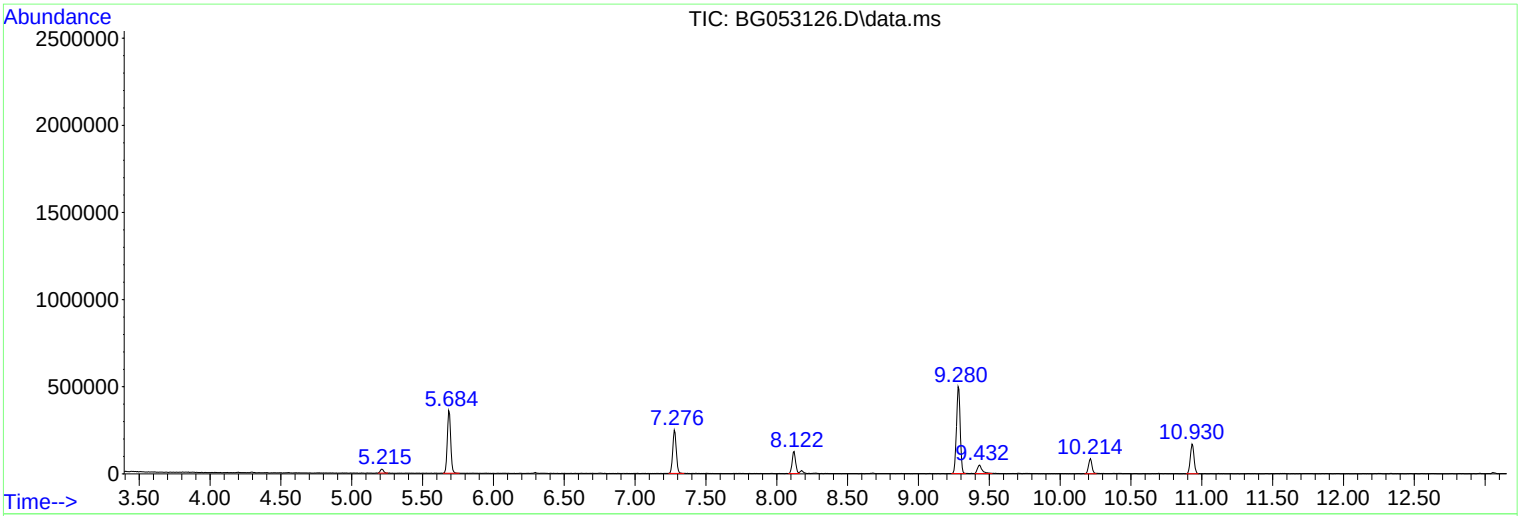
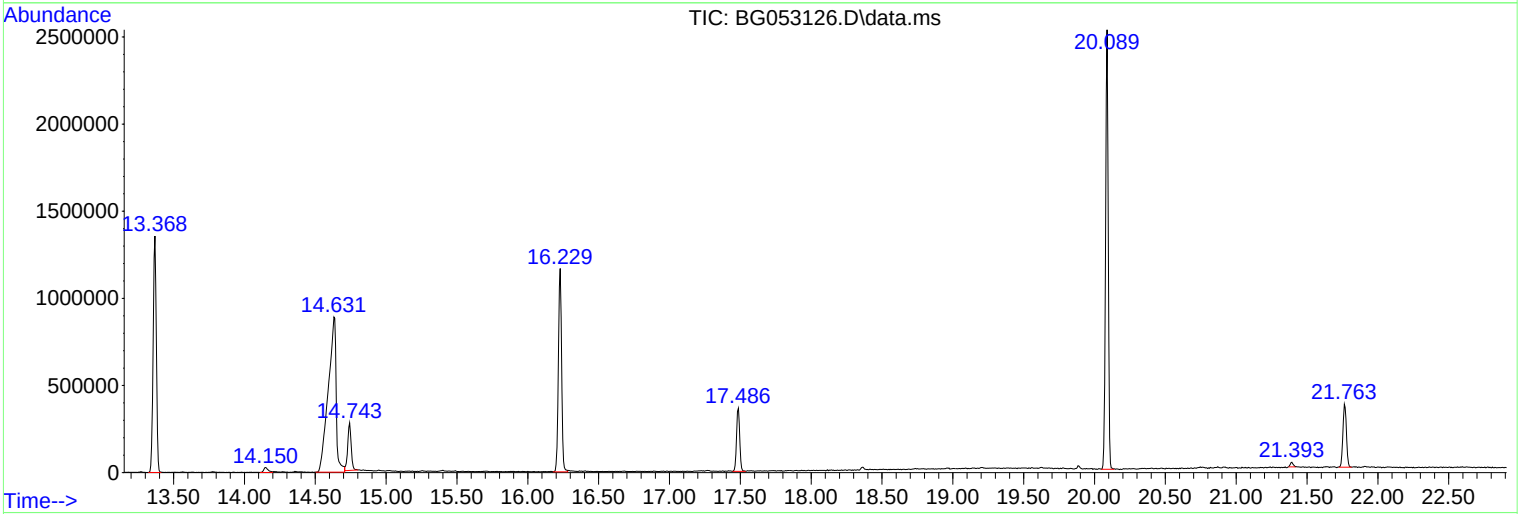
Misc :
ALS Vial : 15 Sample Multiplier: 1

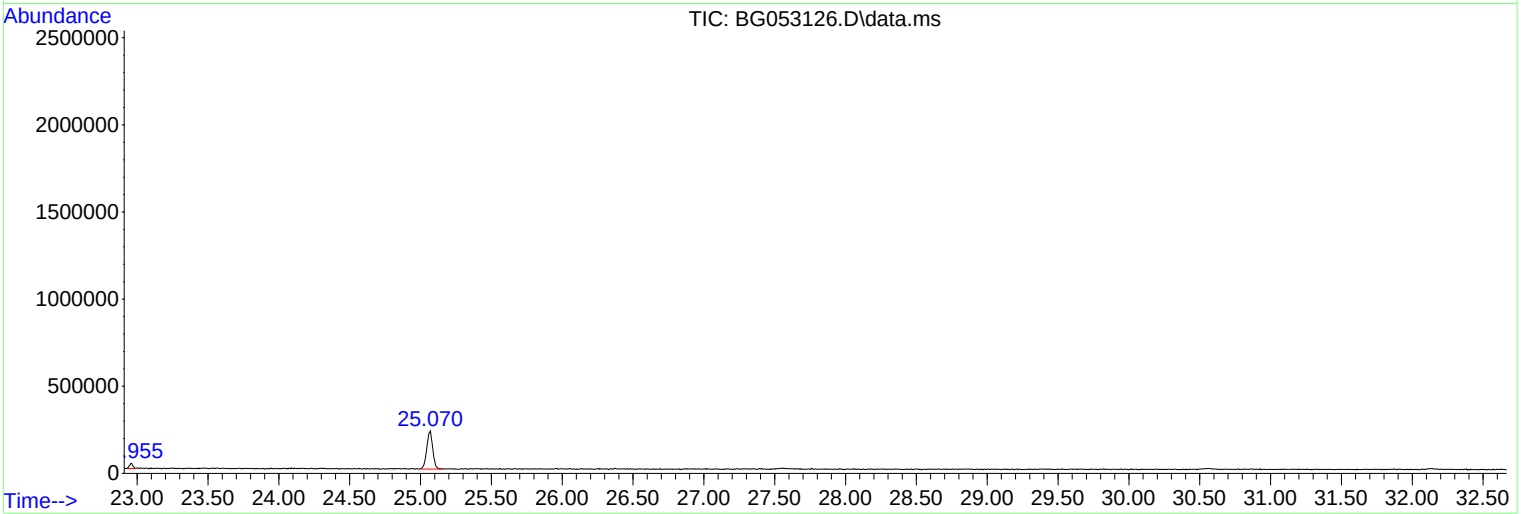
Instrument :
BNA_G
ClientSampleId :
MW-25

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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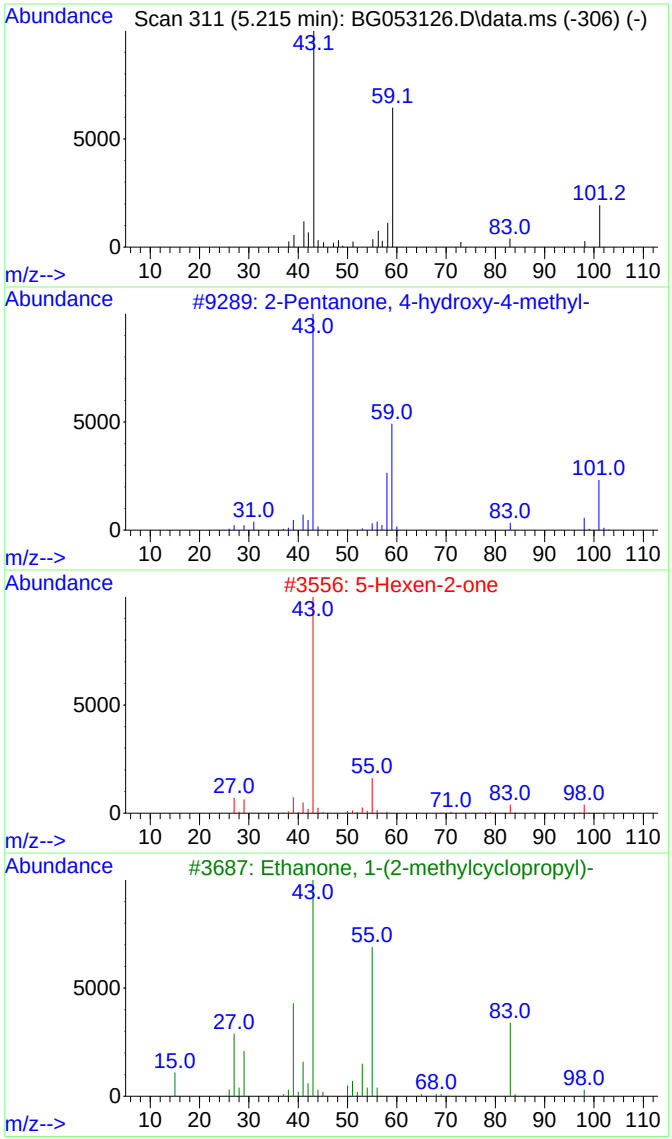
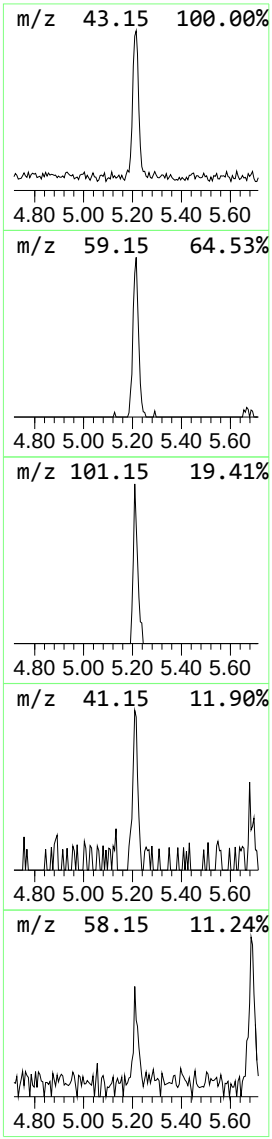
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.215	3.43 ng	37286	1,4-Dichlorobenzene-d4	8.122

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	5-Hexen-2-one	98	C6H10O	000109-49-9	9
3	Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9
4	1,3,4-Oxadiazole, 2-(acetyloxy)-...	172	C7H12N2O3	066398-57-0	9
5	Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	9





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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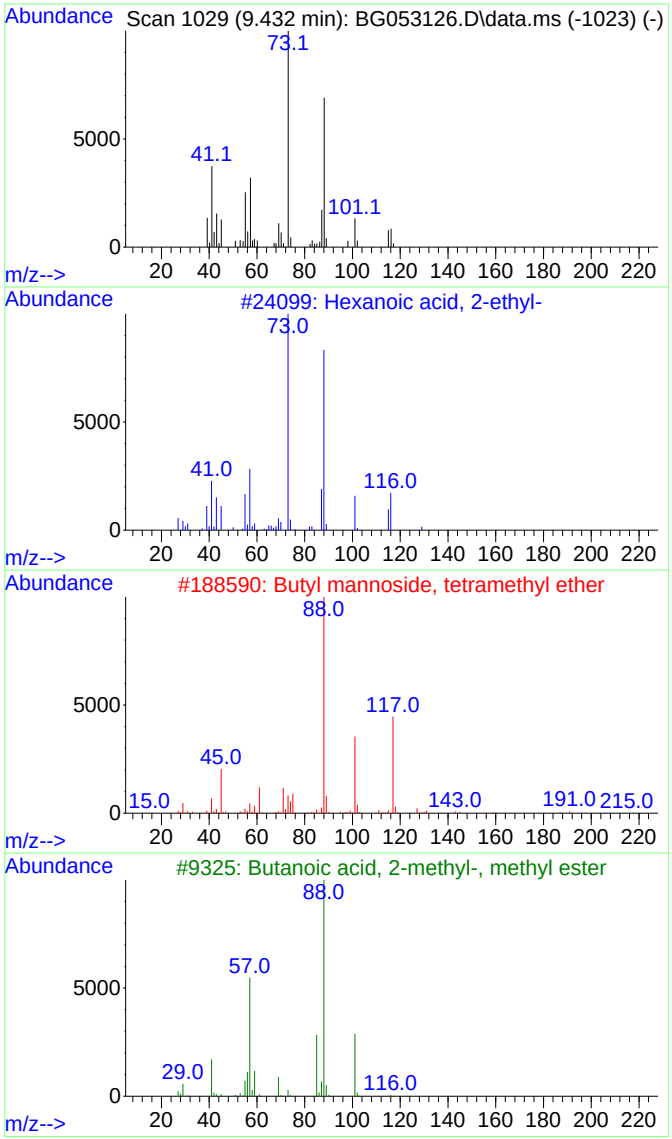
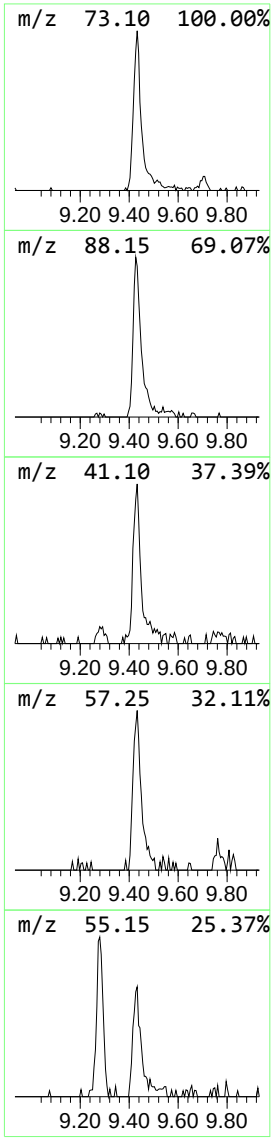
****

Peak Number 2 Hexanoic acid, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.432	10.64 ng	115688	1,4-Dichlorobenzene-d4	8.122

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2	Butyl mannoside, tetramethyl ether	292	C14H28O6	1000501-84-1	50
3	Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	47
4	Hydrazine, 1,2-diethyl-	88	C4H12N2	001615-80-1	47
5	2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	45





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Instrument :
BNA_G
ClientSampleId :
MW-25

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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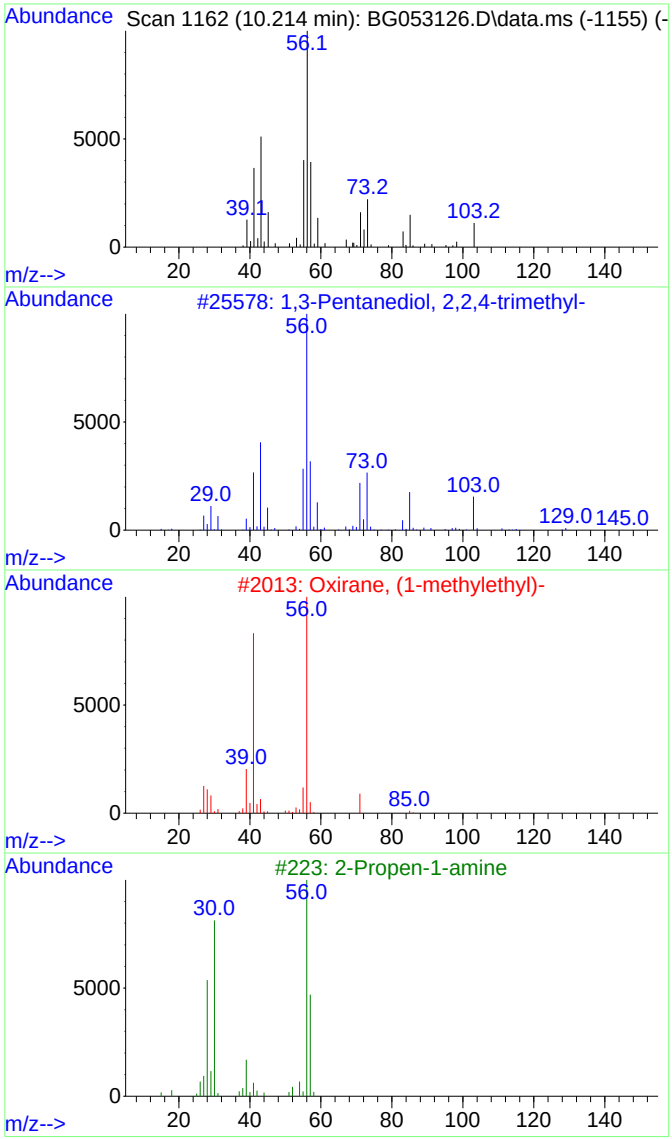
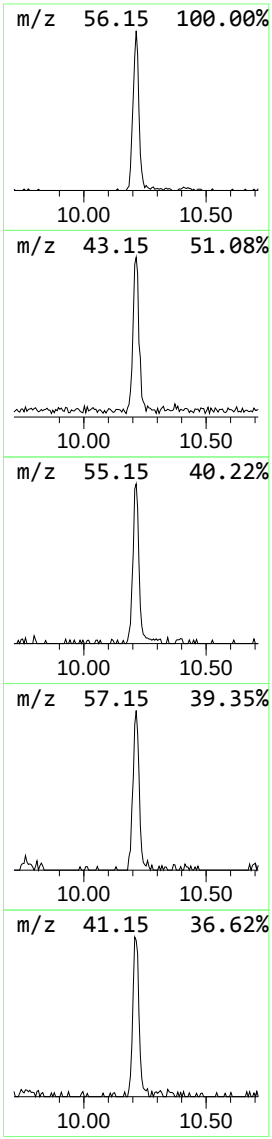
****
Peak Number 3 1,3-Pentanediol, 2,2,4-trim... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.214	9.55 ng	147046	Naphthalene-d8	10.930

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	90
2	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	49
3	2-Propen-1-amine	57	C3H7N	000107-11-9	37
4	1,3-Hexanediol, 2-ethyl-	146	C8H18O2	000094-96-2	33
5	1-Hexene, 5-methyl-	98	C7H14	003524-73-0	32





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Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
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TIC Library : C:\Database\NIST20.L
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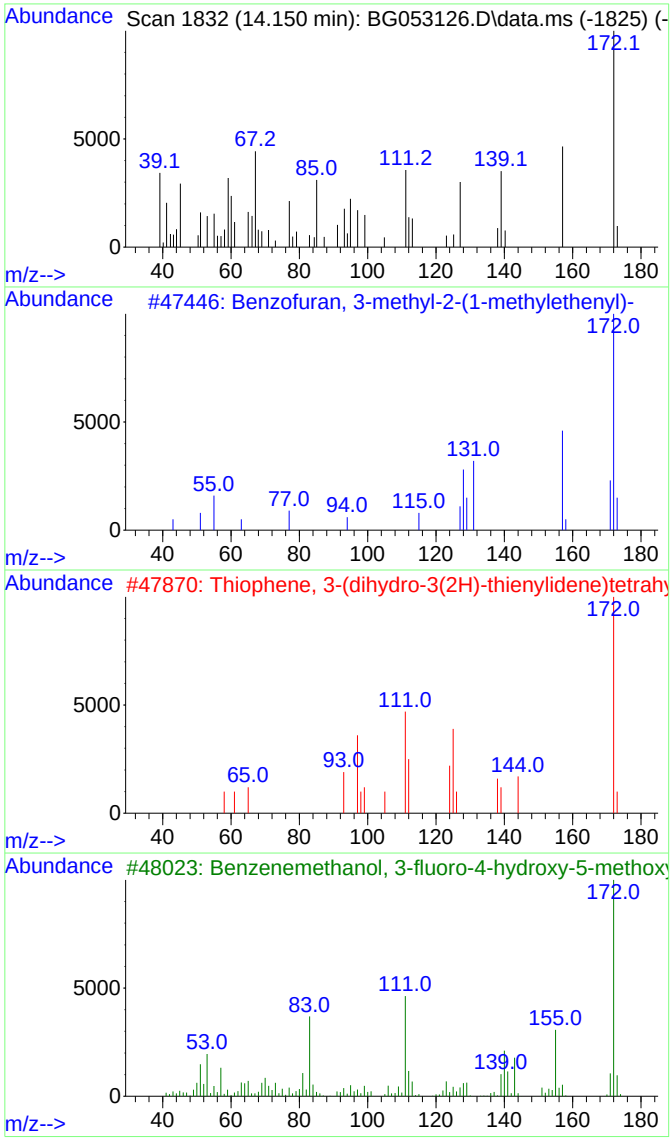
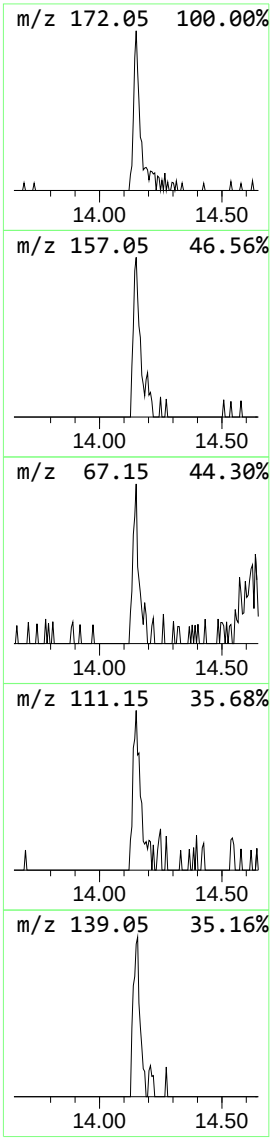
****

Peak Number 4 unknown14.150 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.150	2.73 ng	62986	Acenaphthene-d10	14.743

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzofuran, 3-methyl-2-(1-methyl...	172	C12H12O	023911-58-2	16
2	Thiophene, 3-(dihydro-3(2H)-thie...	172	C8H12S2	040697-97-0	14
3	Benzenemethanol, 3-fluoro-4-hydr...	172	C8H9FO3	099387-76-5	12
4	Benzaldehyde, 2,6-difluoro-3-met...	172	C8H6F2O2	149949-30-4	12
5	5-Cyano-4,5-dihydro-3-phenylisox...	172	C10H8N2O	001011-38-7	10





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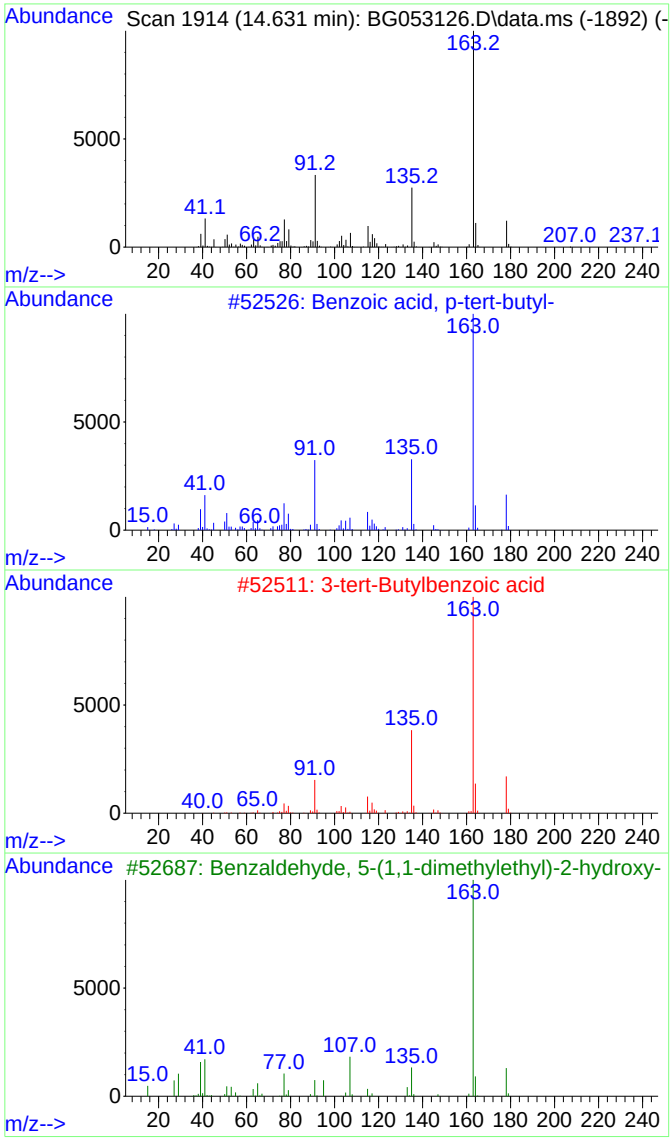
TIC Integration Parameters: LSCINT.P

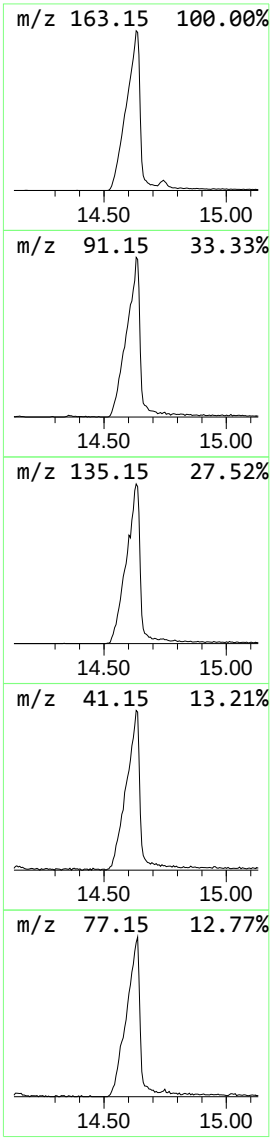
****

Peak Number 5 Benzoic acid, p-tert-butyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.631	150.67 ng	3478990	Acenaphthene-d10	14.743

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	96
2	3-tert-Butylbenzoic acid	178	C11H14O2	007498-54-6	87
3	Benzaldehyde, 5-(1,1-dimethyleth...	178	C11H14O2	002725-53-3	64
4	6-tert-Butyl-2,4-dimethylphenol	178	C12H18O	001879-09-0	64
5	Benzoic acid, 4-acetyl-, methyl ...	178	C10H10O3	003609-53-8	64





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	3.4	ng	37286	1	8.122	217490	20.0
Hexanoic acid, ...	9.432	10.6	ng	115688	1	8.122	217490	20.0
1,3-Pentanediol...	10.214	9.6	ng	147046	2	10.930	307890	20.0
unknown14.150	14.150	2.7	ng	62986	3	14.743	461790	20.0
Benzoic acid, p...	14.631	150.7	ng	3478990	3	14.743	461790	20.0