LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052322\
Data File : BG053666.D
Acq On : 23 May 2022 16:10
Operator : CG/JU
Sample : N2968-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-40

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-BG050522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053666.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.743	54	60	67	rBV	46451	75520	2.93%	0.665%
2	4.465	175	183	189	rBV3	23107	48340	1.87%	0.425%
3	4.536	189	195	196	rVV4	19832	34522	1.34%	0.304%
4	4.553	196	198	212	rVB	22518	31748	1.23%	0.279%
5	5.628	375	381	391	rBV	250798	420658	16.32%	3.702%
6	7.232	647	654	664	rBV	158708	324687	12.59%	2.857%
7	8.060	788	795	802	rBV	106646	186316	7.23%	1.640%
8	8.366	844	847	855	rBV3	36913	66053	2.56%	0.581%
9	9.112	962	974	980	rBV5	76665	334504	12.97%	2.944%
10	9.223	980	993	1001	rVB2	422735	1119307	43.41%	9.850%
11	9.852	1088	1100	1111	rBV2	44702	101265	3.93%	0.891%
12	10.868	1264	1273	1281	rBV	151562	283420	10.99%	2.494%
13	13.312	1679	1689	1696	rVB	1126456	1804898	70.00%	15.883%
14	13.729	1757	1760	1767	rBV3	16587	39619	1.54%	0.349%
15	14.352	1861	1866	1871	rBV7	14313	27037	1.05%	0.238%
16	14.528	1892	1896	1900	rBV3	14795	25828	1.00%	0.227%
17	14.687	1913	1923	1930	rBV	255849	434140	16.84%	3.820%
18	16.179	2170	2177	2186	rBV	999058	1531757	59.41%	13.479%
19	17.436	2385	2391	2396	rBV	323296	494803	19.19%	4.354%
20	18.323	2537	2542	2549	rBV2	74959	136878	5.31%	1.205%
21	19.586	2753	2757	2763	rBV5	36773	62266	2.42%	0.548%
22	20.038	2828	2834	2841	rBV	1975992	2578295	100.00%	22.689%
23	21.337	3051	3055	3061	rBV2	65659	110880	4.30%	0.976%
24	21.712	3112	3119	3127	rBV	313595	540218	20.95%	4.754%
25	24.973	3664	3674	3685	rVB	191022	550921	21.37%	4.848%

Sum of corrected areas: 11363880

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Misc :
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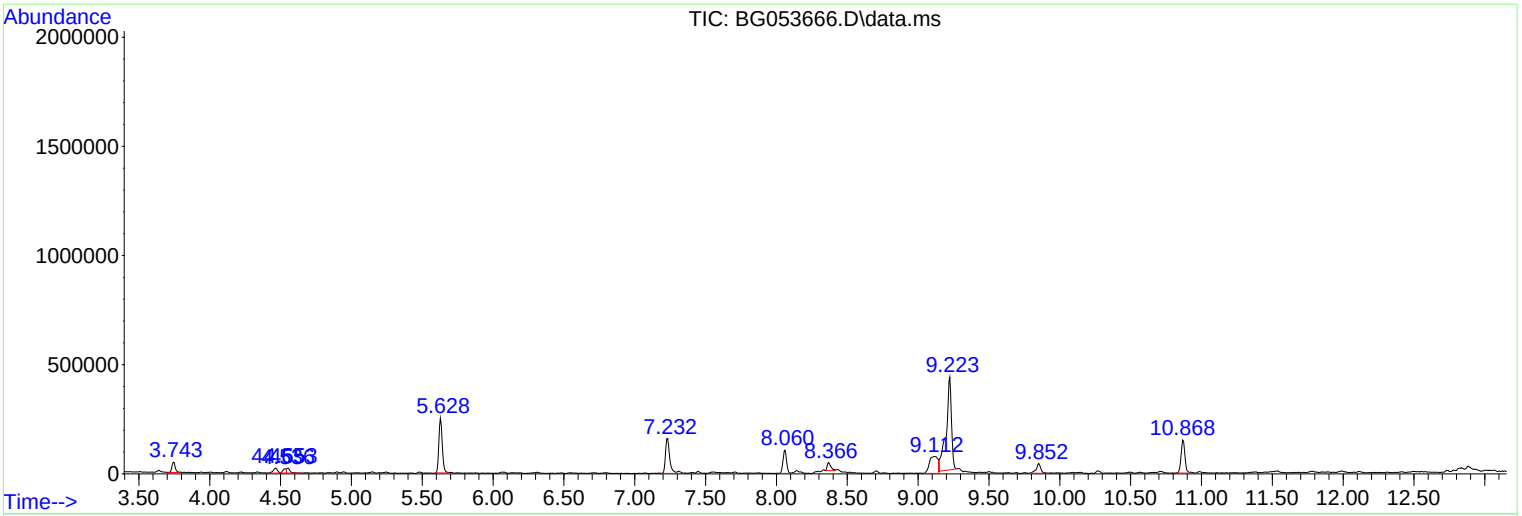
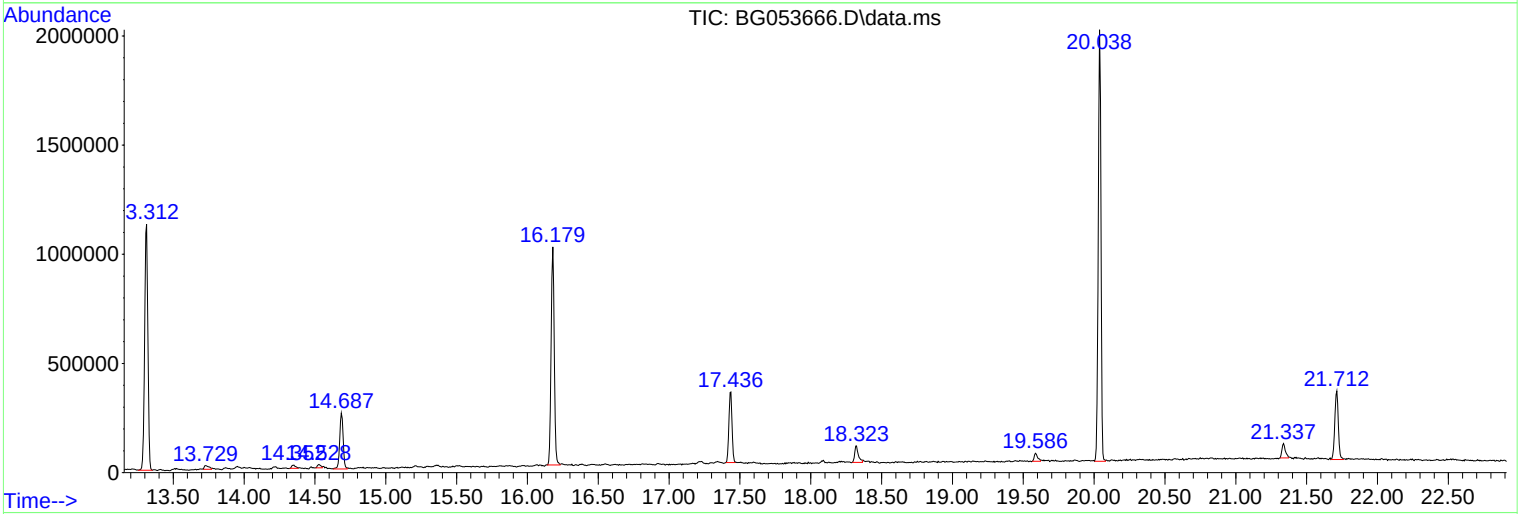
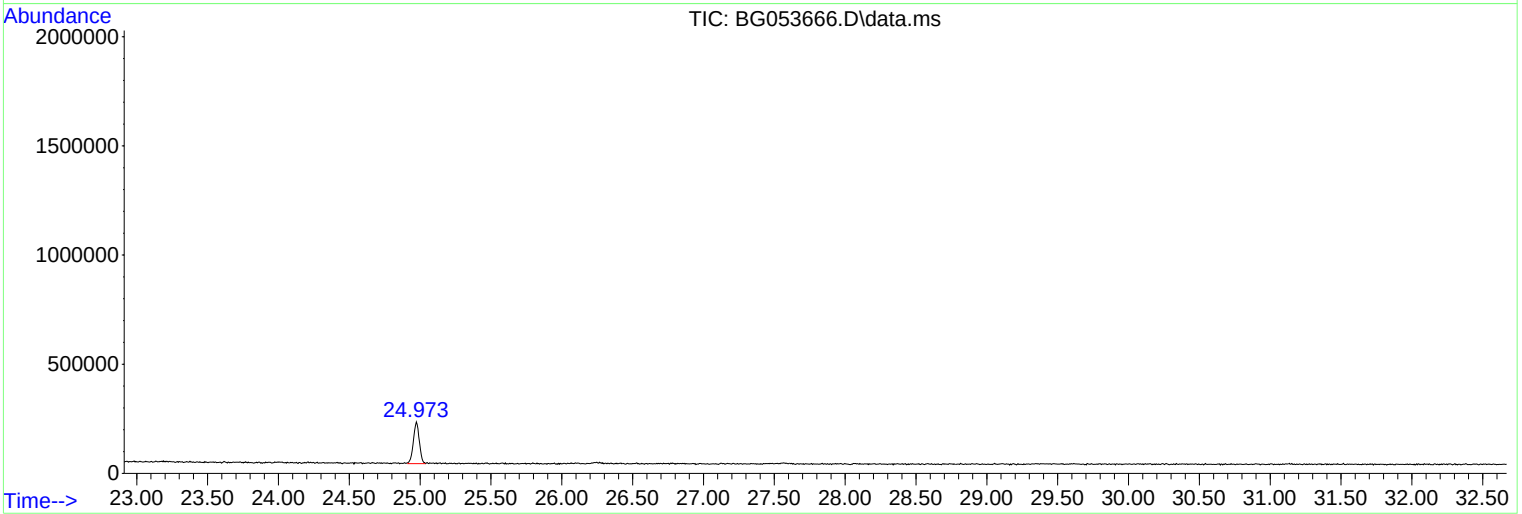
Instrument :
BNA_G
ClientSampleId :
MW-40

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.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 : BG053666.D
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Instrument :
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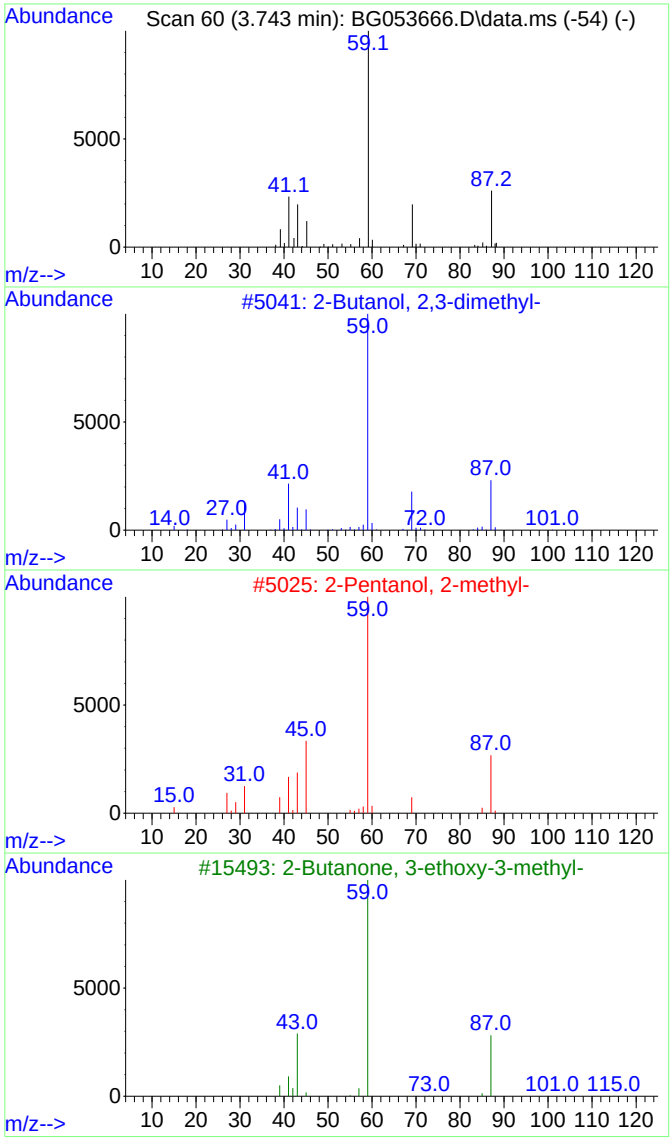
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

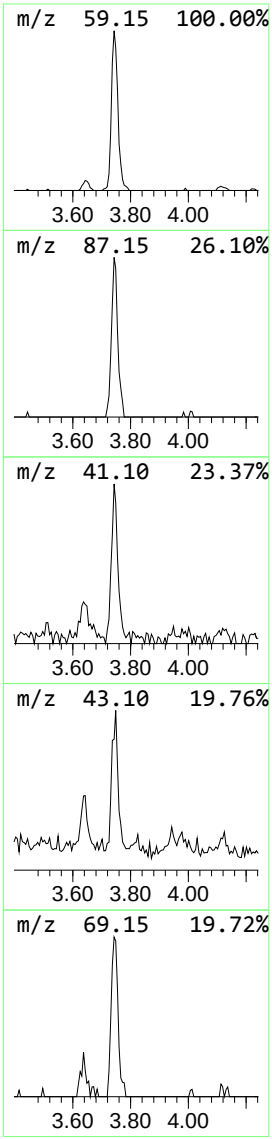
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Butanol, 2,3-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.743	8.11 ng	75520	1,4-Dichlorobenzene-d4	8.060

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	78
2	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	40
3	2-Butanone, 3-ethoxy-3-methyl-	130	C7H14O2	036687-99-7	39
4	Propane, 1-ethoxy-	88	C5H12O	000628-32-0	38
5	N-Formyl-d-threo-O-methylthreonine	161	C6H11NO4	1000214-69-5	36





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Data File : BG053666.D
Acq On : 23 May 2022 16:10
Operator : CG/JU
Sample : N2968-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-40

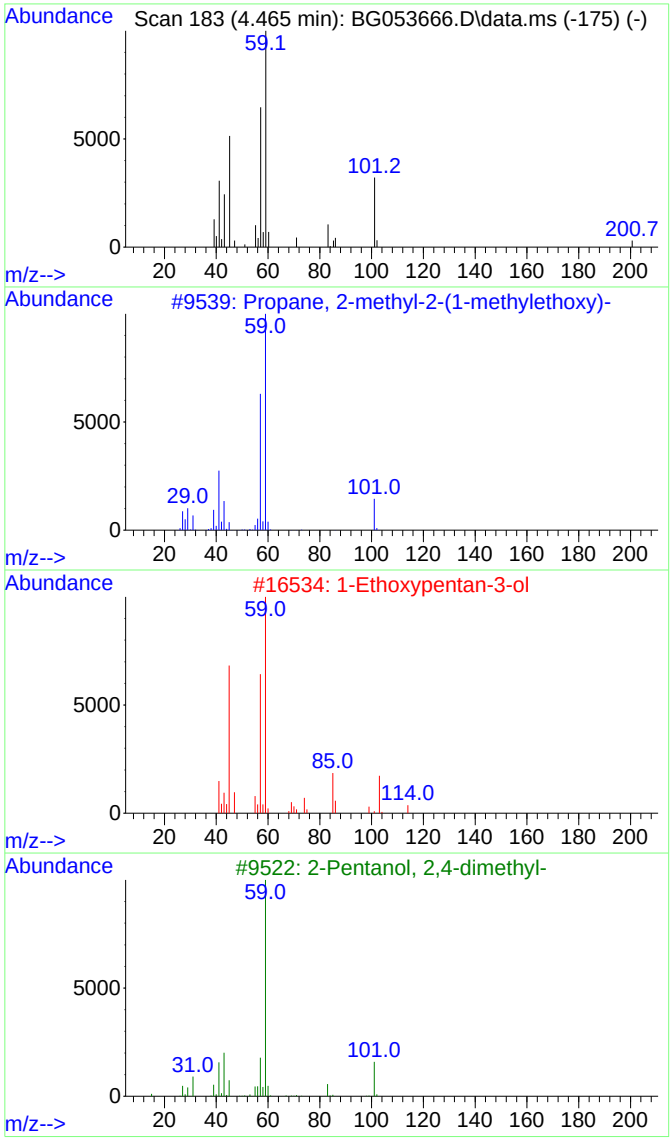
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

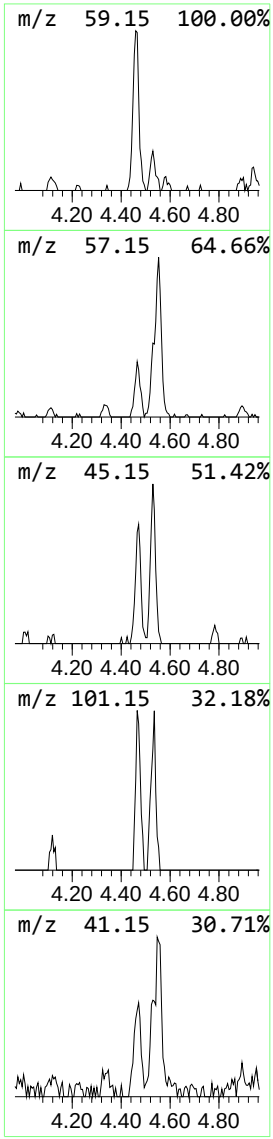
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Propane, 2-methyl-2-(1-meth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.465	5.19 ng	48340	1,4-Dichlorobenzene-d4	8.060

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
2	1-Ethoxypentan-3-ol	132	C7H16O2	100910-92-7	45
3	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	42
4	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	36
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	36





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052322\
Data File : BG053666.D
Acq On : 23 May 2022 16:10
Operator : CG/JU
Sample : N2968-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-40

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
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TIC Library : C:\Database\NIST20.L
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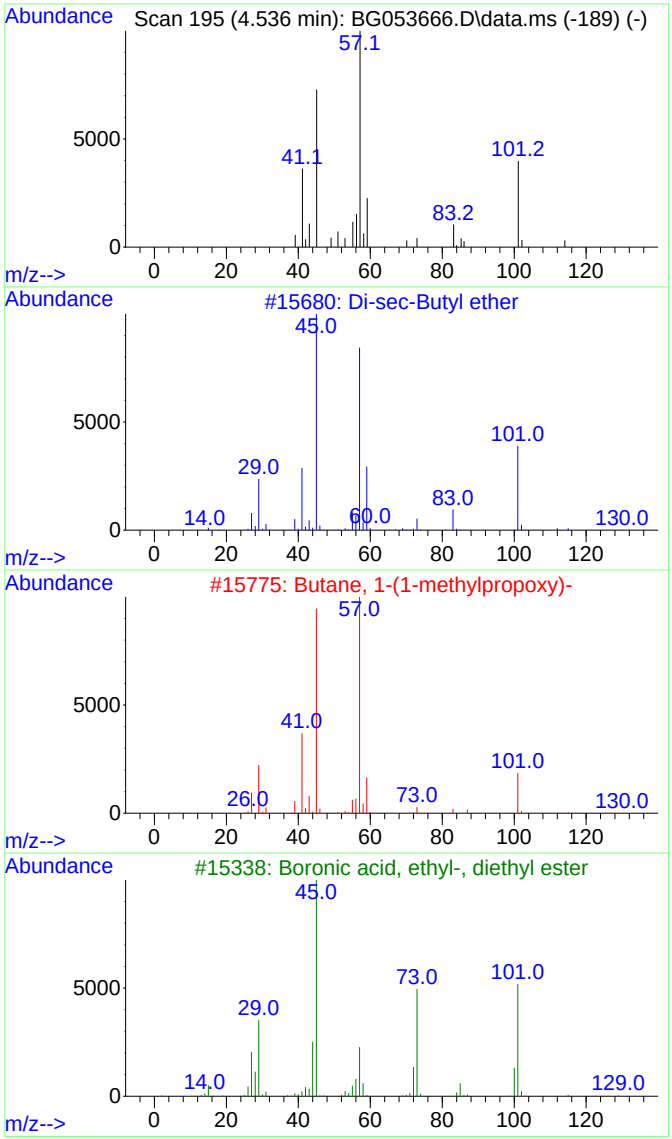
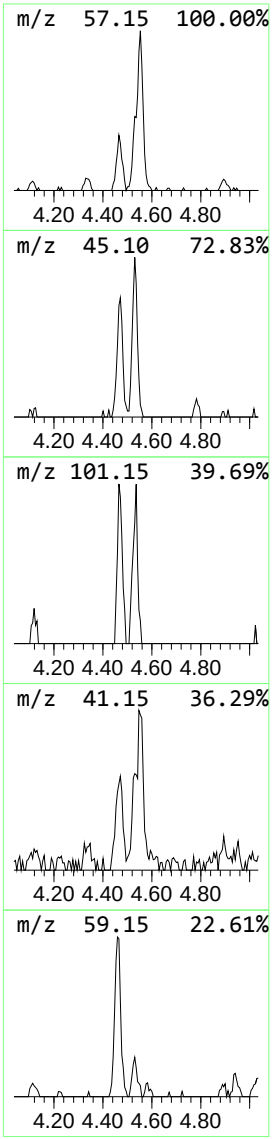
****

Peak Number 3 unknown4.536 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.536	3.71 ng	34522	1,4-Dichlorobenzene-d4	8.060

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-sec-Butyl ether	130	C8H18O	006863-58-7	42
2	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	40
3	Boronic acid, ethyl-, diethyl ester	130	C6H15BO2	053907-92-9	38
4	4-Methyl-2-hexanol	116	C7H16O	002313-61-3	32
5	Sulfurous acid, isobutyl 2-methy...	238	C10H22O4S	1000309-20-3	28





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052322\
Data File : BG053666.D
Acq On : 23 May 2022 16:10
Operator : CG/JU
Sample : N2968-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-40

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

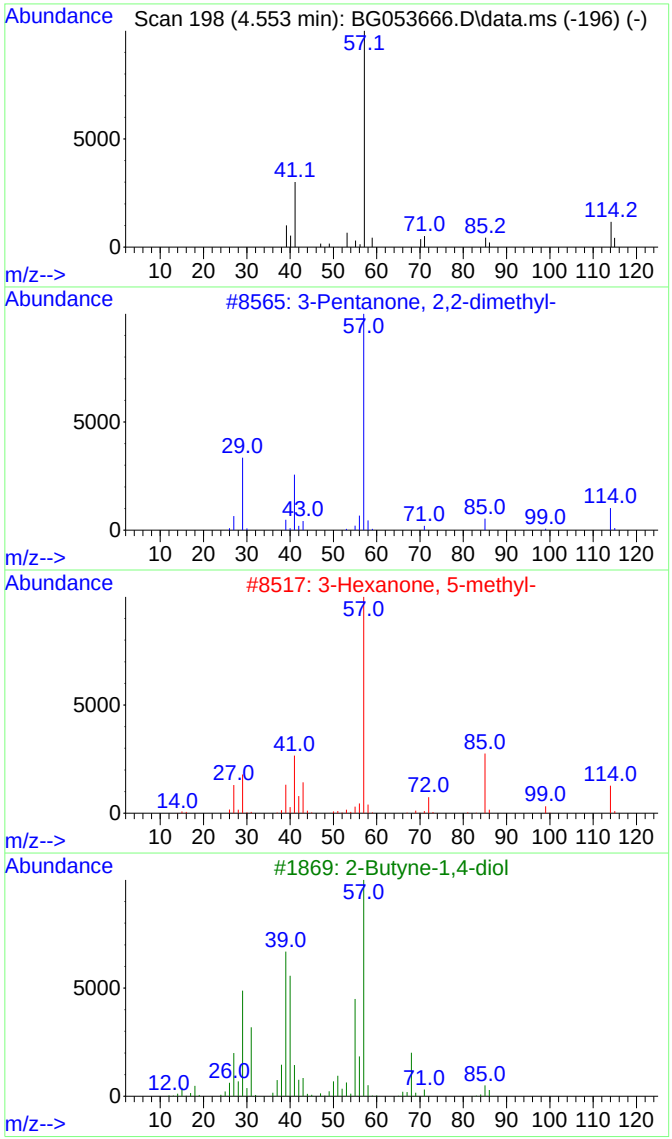
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

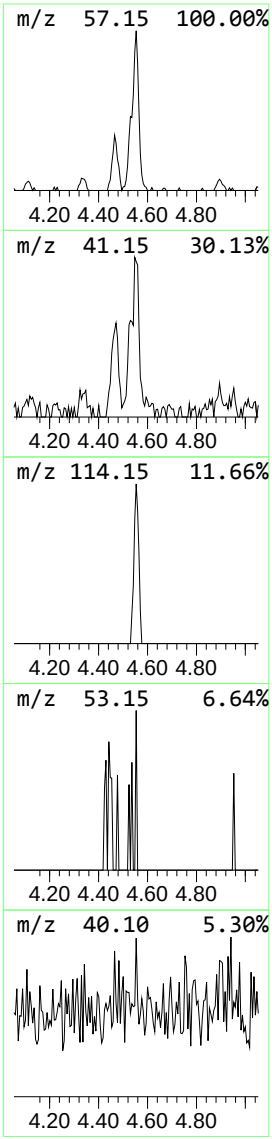
****

Peak Number 4 unknown4.553 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.553	3.41 ng	31748	1,4-Dichlorobenzene-d4	8.060

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone, 2,2-dimethyl-	114	C7H14O	000564-04-5	38
2	3-Hexanone, 5-methyl-	114	C7H14O	000623-56-3	32
3	2-Butyne-1,4-diol	86	C4H6O2	000110-65-6	23
4	3-Heptanone	114	C7H14O	000106-35-4	23
5	1,2,2-Trimethylpropyl trifluoroa...	198	C8H13F3O2	116465-21-5	9





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Data File : BG053666.D
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Operator : CG/JU
Sample : N2968-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-40

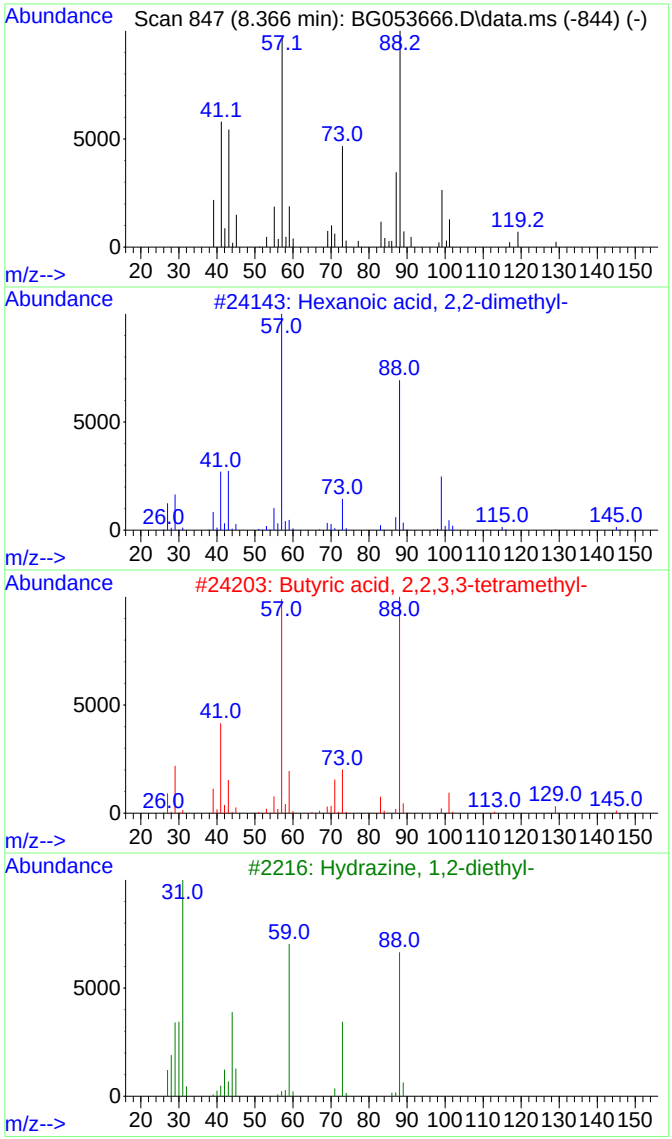
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

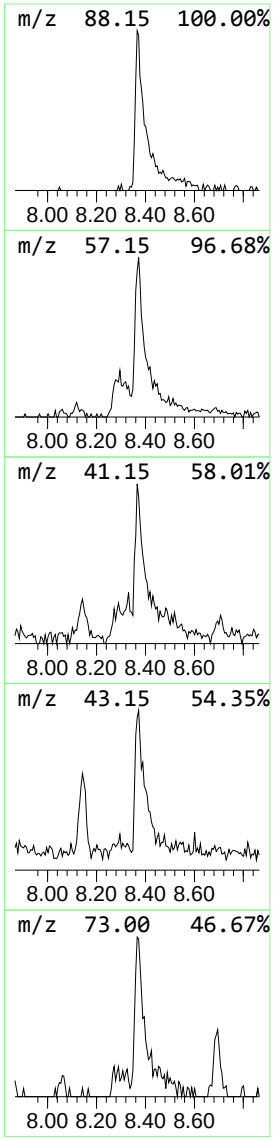
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Hexanoic acid, 2,2-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.366	7.09 ng	66053	1,4-Dichlorobenzene-d4	8.060

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2,2-dimethyl-	144	C8H16O2	000813-72-9	50
2	Butyric acid, 2,2,3,3-tetramethyl-	144	C8H16O2	030407-41-1	45
3	Hydrazine, 1,2-diethyl-	88	C4H12N2	001615-80-1	43
4	Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	42
5	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	40





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TIC Library : C:\Database\NIST20.L
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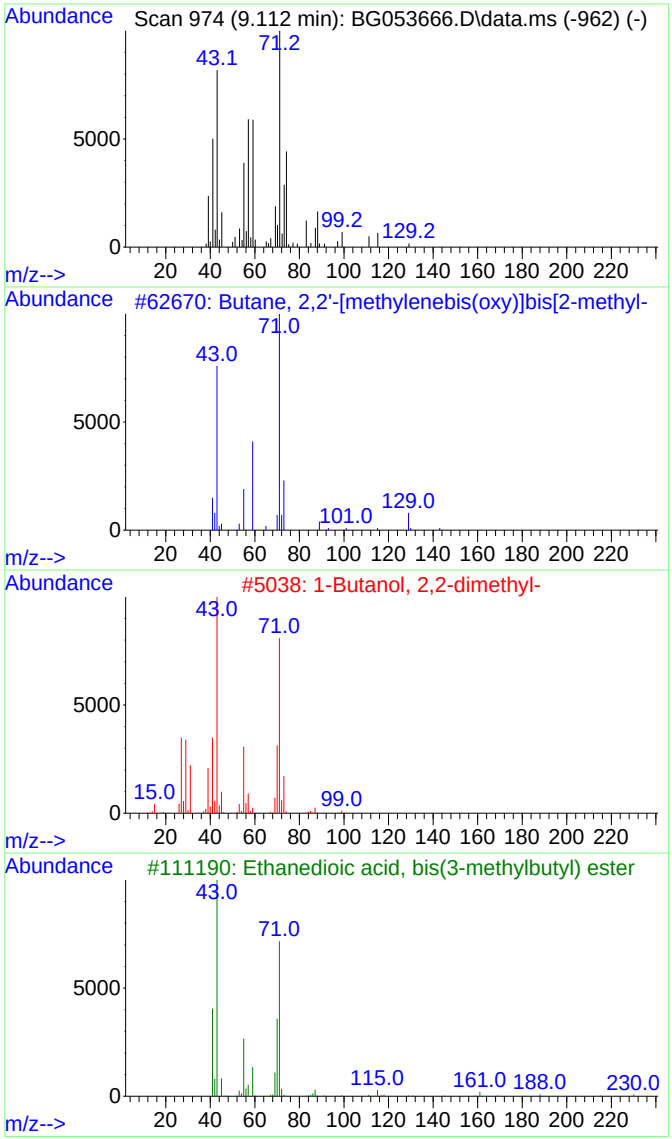
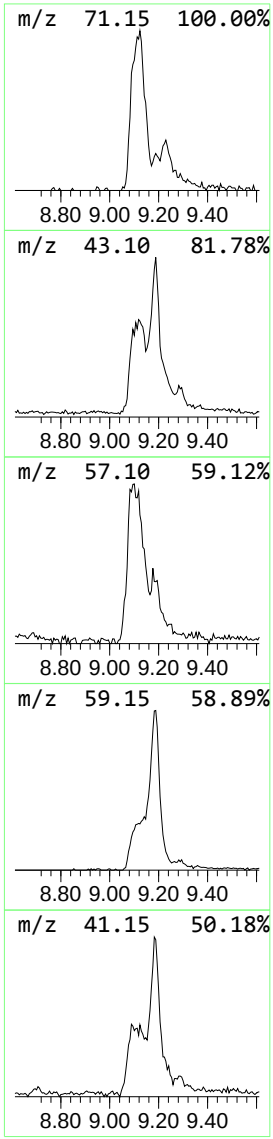
****
Peak Number 6 Butane, 2,2'-[methylenebis(... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.112	35.91 ng	334504	1,4-Dichlorobenzene-d4	8.060

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,2'-[methylenebis(oxy)]...	188	C11H24O2	054699-28-4	50
2	1-Butanol, 2,2-dimethyl-	102	C6H14O	001185-33-7	35
3	Ethanedioic acid, bis(3-methylbu...	230	C12H22O4	002051-00-5	35
4	3-Hexanol, 4,4-dimethyl-	130	C8H18O	019550-09-5	35
5	4,4-Dimethyl-1-hexene	112	C8H16	001647-08-1	27





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Sample : N2968-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
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TIC Library : C:\Database\NIST20.L
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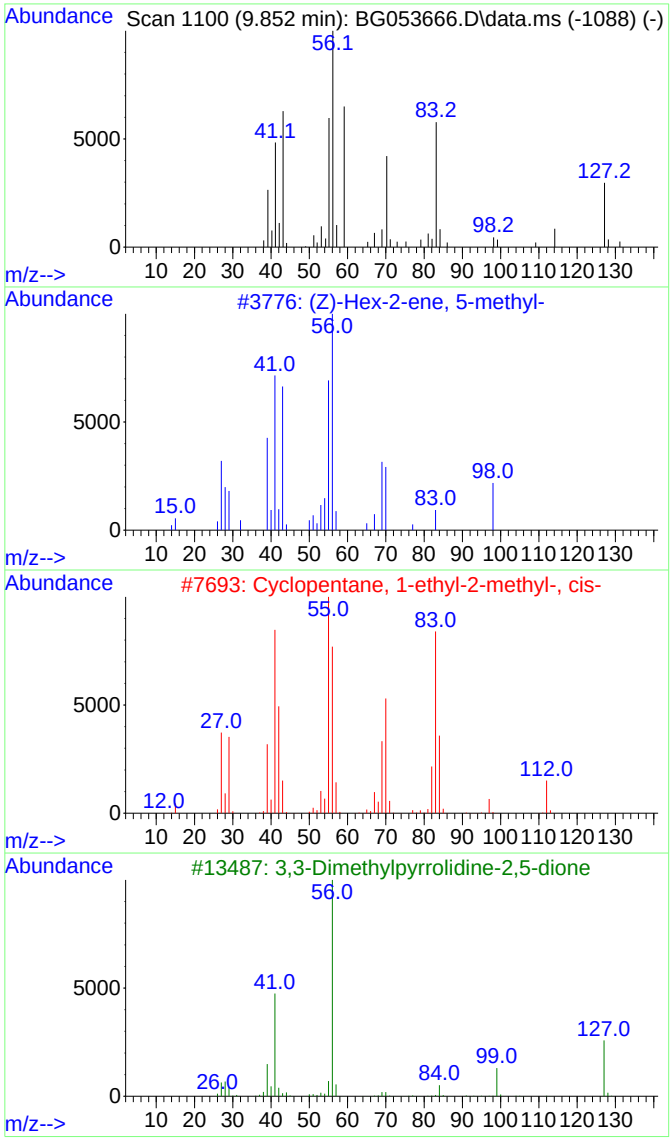
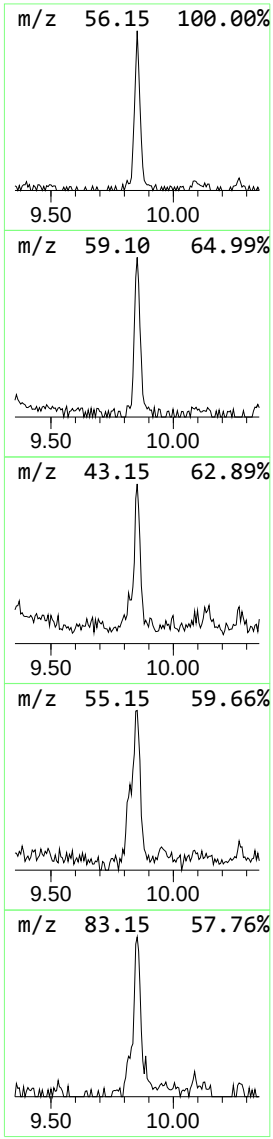
****

Peak Number 7 unknown9.852 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.852	7.15 ng	101265	Naphthalene-d8	10.868

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(Z)-Hex-2-ene, 5-methyl-	98	C7H14	013151-17-2	35
2	Cyclopentane, 1-ethyl-2-methyl-,...	112	C8H16	000930-89-2	35
3	3,3-Dimethylpyrrolidine-2,5-dione	127	C6H9NO2	003437-29-4	35
4	1-Hexene, 5-methyl-	98	C7H14	003524-73-0	27
5	1-Hexene, 2-methyl-	98	C7H14	006094-02-6	25





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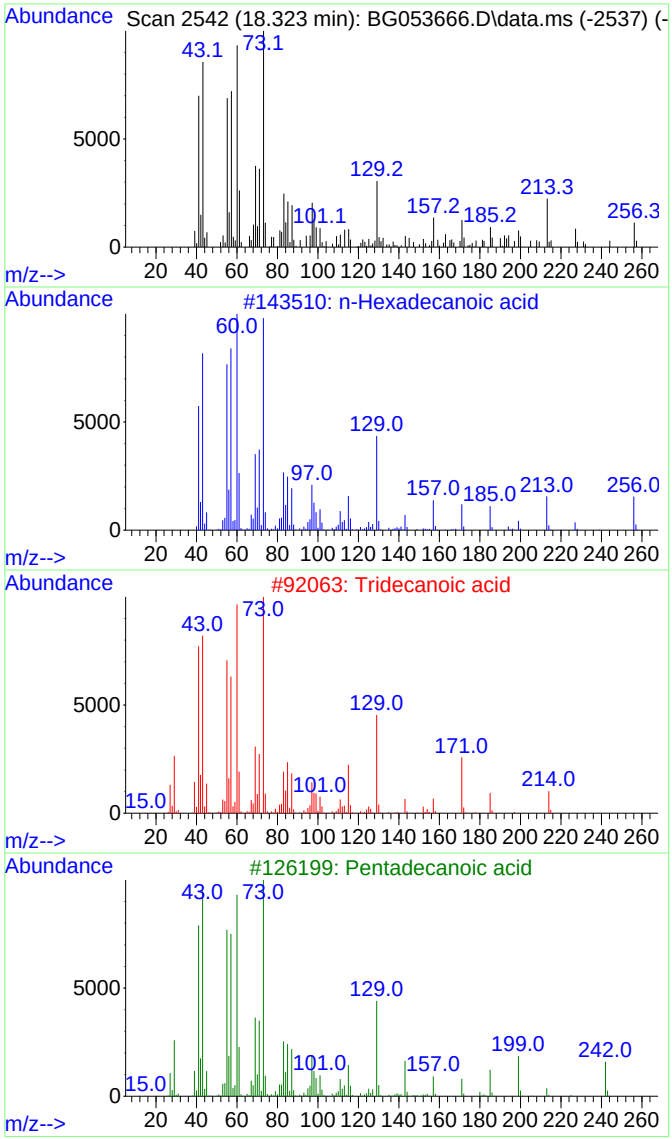
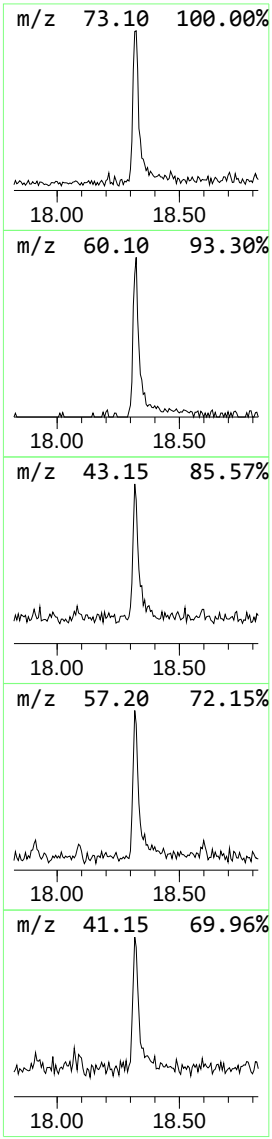
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.323	5.53 ng	136878	Phenanthrene-d10	17.436

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
5	Undecanoic acid	186	C11H22O2	000112-37-8	68





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Operator : CG/JU
Sample : N2968-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-40

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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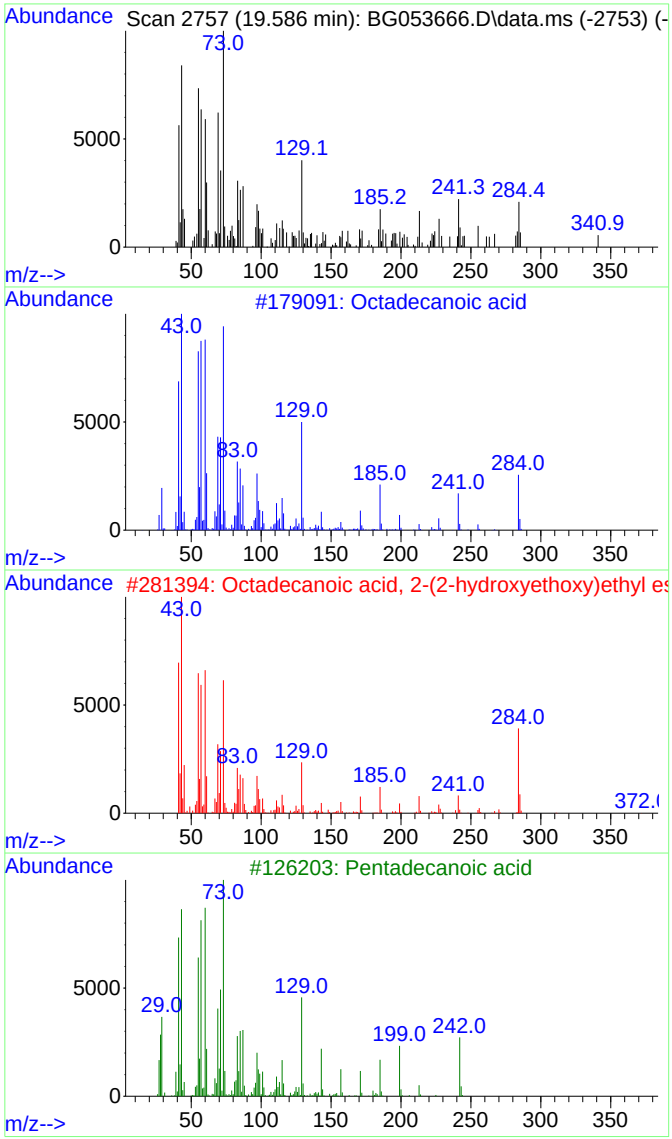
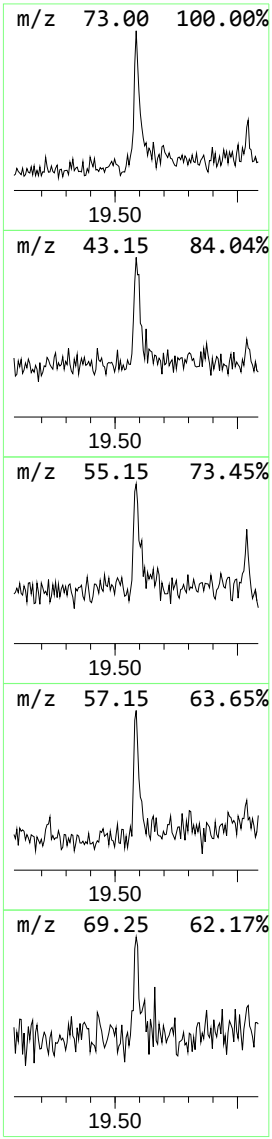
****

Peak Number 9 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.586	2.31 ng	62266	Chrysene-d12	21.712

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	59
4	Undecanoic acid	186	C11H22O2	000112-37-8	43
5	Methyl 2,6-anhydro-.alpha.-d-alt...	176	C7H12O5	1000130-02-0	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052322\
Data File : BG053666.D
Acq On : 23 May 2022 16:10
Operator : CG/JU
Sample : N2968-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-40

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

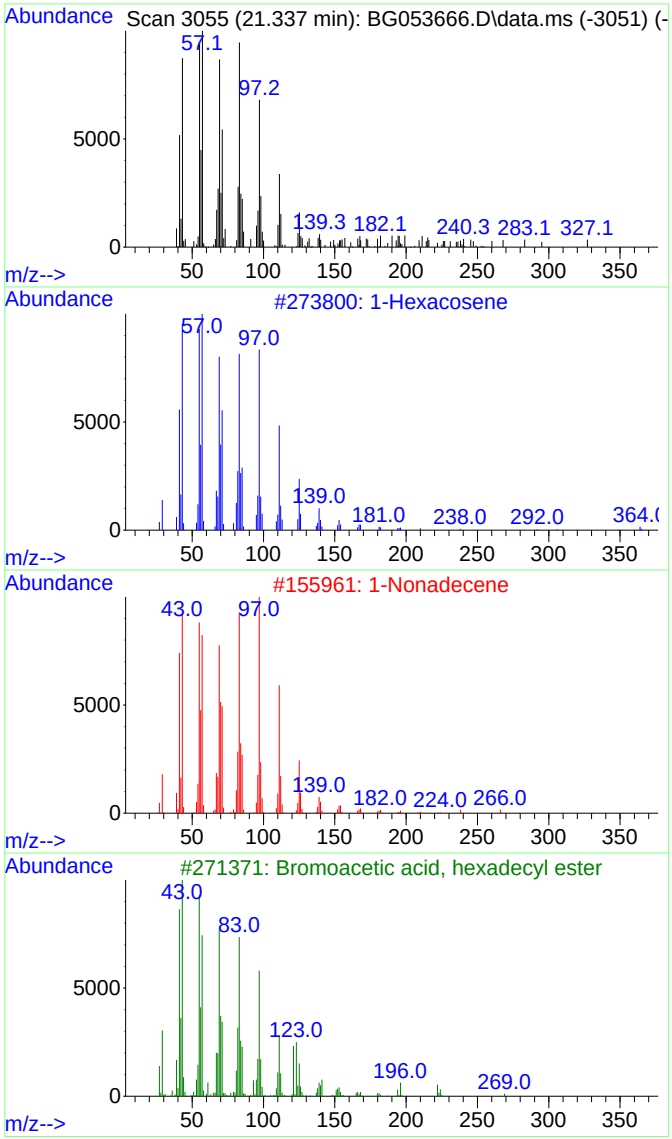
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

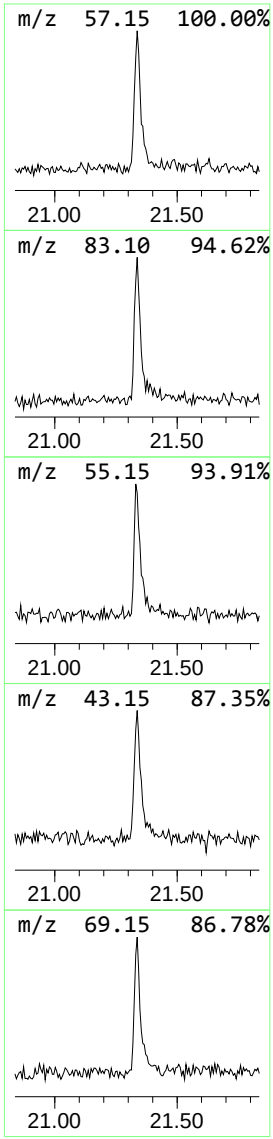
****

Peak Number 10 1-Hexacosene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.337	4.11 ng	110880	Chrysene-d12	21.712

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene	364	C26H52	018835-33-1	94
2	1-Nonadecene	266	C19H38	018435-45-5	91
3	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	90
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	90
5	1-Heptadecene	238	C17H34	006765-39-5	89





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052322\
Data File : BG053666.D
Acq On : 23 May 2022 16:10
Operator : CG/JU
Sample : N2968-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-40

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.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-Butanol, 2,3-...	3.743	8.1	ng	75520	1	8.060	186316	20.0
Propane, 2-meth...	4.465	5.2	ng	48340	1	8.060	186316	20.0
unknown4.536	4.536	3.7	ng	34522	1	8.060	186316	20.0
unknown4.553	4.553	3.4	ng	31748	1	8.060	186316	20.0
Hexanoic acid, ...	8.366	7.1	ng	66053	1	8.060	186316	20.0
Butane, 2,2'-[m...	9.112	35.9	ng	334504	1	8.060	186316	20.0
unknown9.852	9.852	7.2	ng	101265	2	10.868	283420	20.0
n-Hexadecanoic ...	18.323	5.5	ng	136878	4	17.436	494803	20.0
Octadecanoic acid	19.586	2.3	ng	62266	5	21.712	540218	20.0
1-Hexacosene	21.337	4.1	ng	110880	5	21.712	540218	20.0