LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
Data File : BG053357.D
Acq On : 28 Apr 2022 2:36
Operator : CG/JU
Sample : N2482-10
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-15

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: BG053357.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.551	192	198	208	rVB	74248	116242	3.32%	0.928%
2	5.192	300	307	315	rBV2	28963	47294	1.35%	0.378%
3	5.667	382	388	399	rVB	396911	661722	18.89%	5.282%
4	7.265	653	660	673	rVB	299417	536687	15.32%	4.284%
5	7.630	715	722	726	rBV	41239	64067	1.83%	0.511%
6	7.682	726	731	738	rVB	41026	64491	1.84%	0.515%
7	7.870	756	763	770	rBV	60157	106747	3.05%	0.852%
8	8.105	792	803	808	rBV	98096	185321	5.29%	1.479%
9	8.158	808	812	819	rVB	44526	74707	2.13%	0.596%
10	9.269	993	1001	1010	rBV	465938	856432	24.44%	6.837%
11	10.913	1273	1281	1288	rBV	134679	242671	6.93%	1.937%
12	13.087	1645	1651	1662	rBV2	53641	93179	2.66%	0.744%
13	13.351	1686	1696	1704	rBV	1195920	1997215	57.01%	15.943%
14	13.569	1727	1733	1739	rBV	195016	303264	8.66%	2.421%
15	14.726	1921	1930	1937	rBV	225442	354415	10.12%	2.829%
16	15.525	2061	2066	2072	rVB	40208	58447	1.67%	0.467%
17	16.065	2152	2158	2167	rVB	41539	56148	1.60%	0.448%
18	16.218	2176	2184	2194	rBV	1024155	1637650	46.74%	13.073%
19	17.469	2391	2397	2403	rBV	290424	454947	12.99%	3.632%
20	20.077	2835	2841	2847	rBV	2609888	3503544	100.00%	27.967%
21	21.757	3120	3127	3134	rVB	320218	558132	15.93%	4.455%
22	25.053	3676	3688	3702	rBV3	184807	553937	15.81%	4.422%

Sum of corrected areas: 12527259

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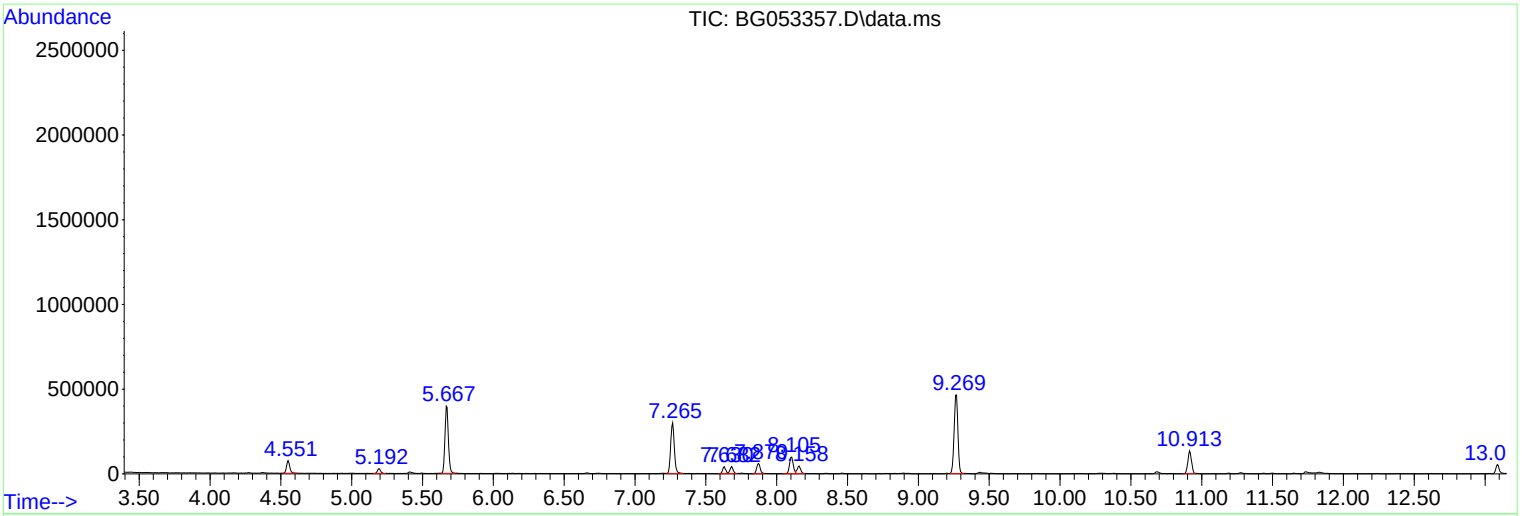
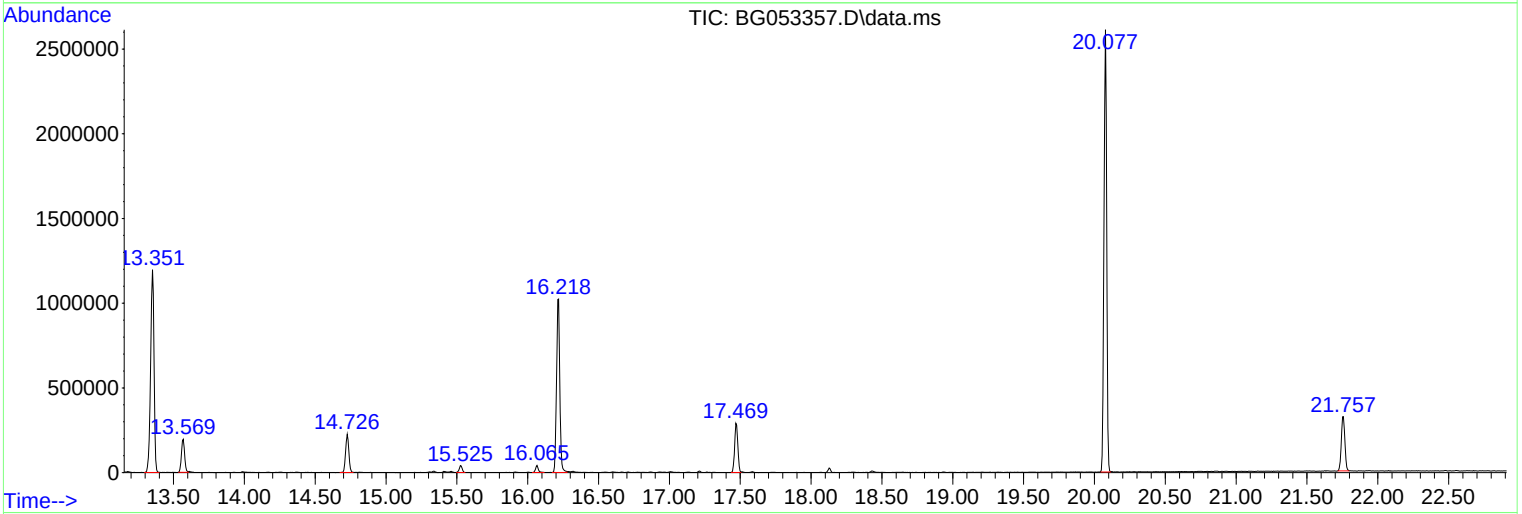
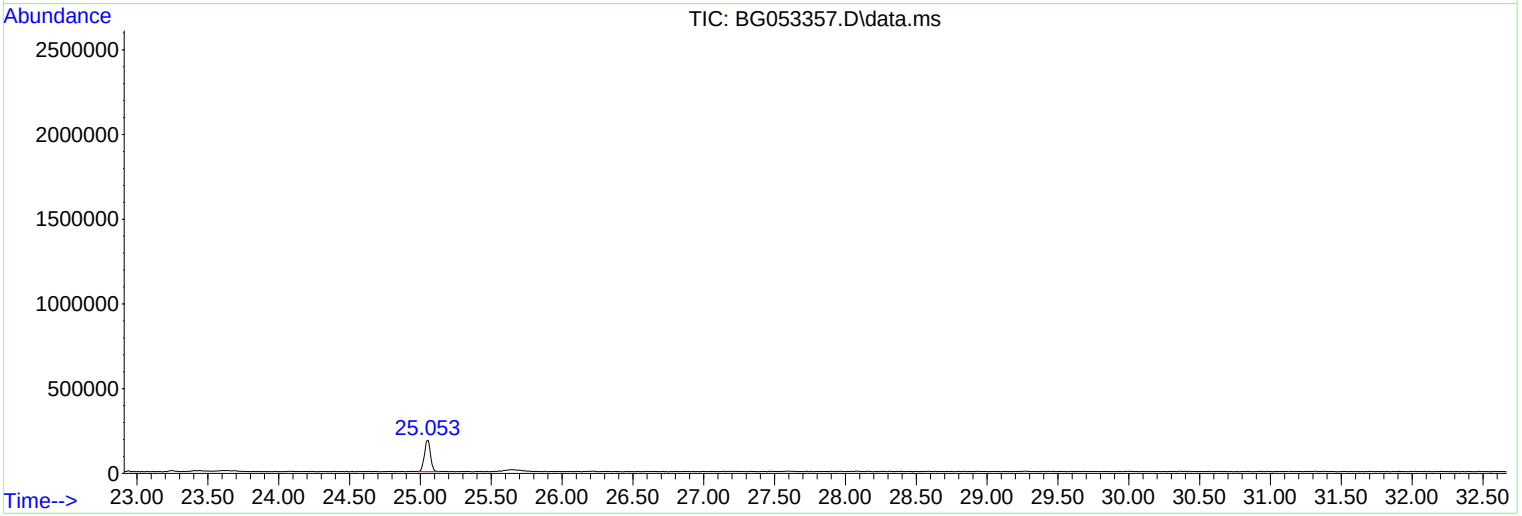
MW-15

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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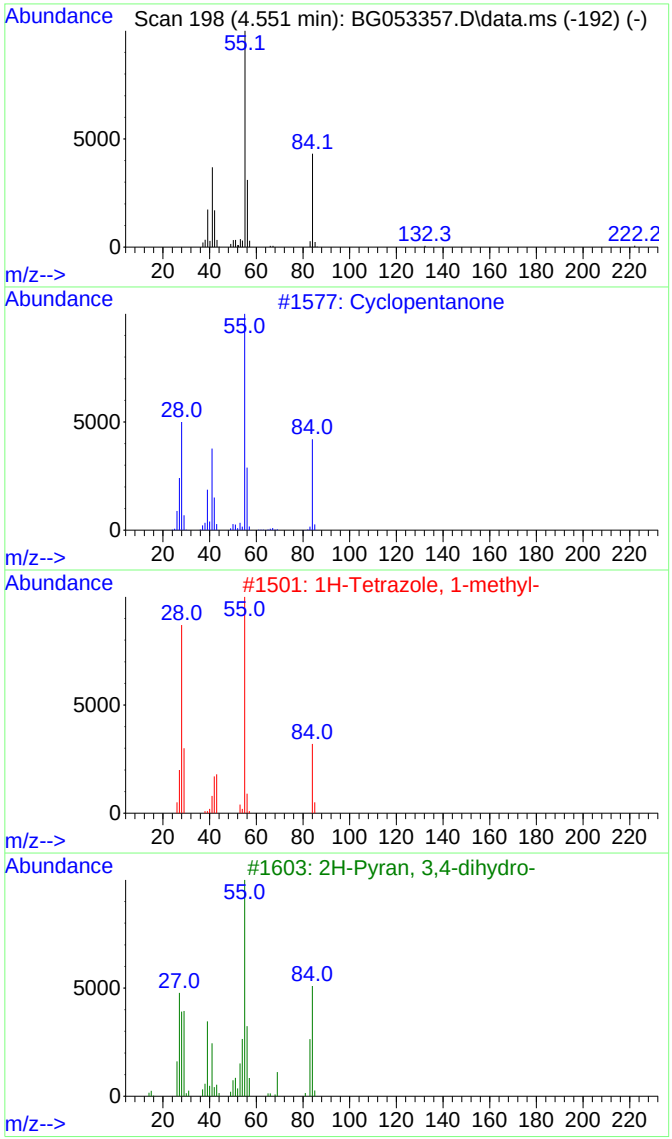
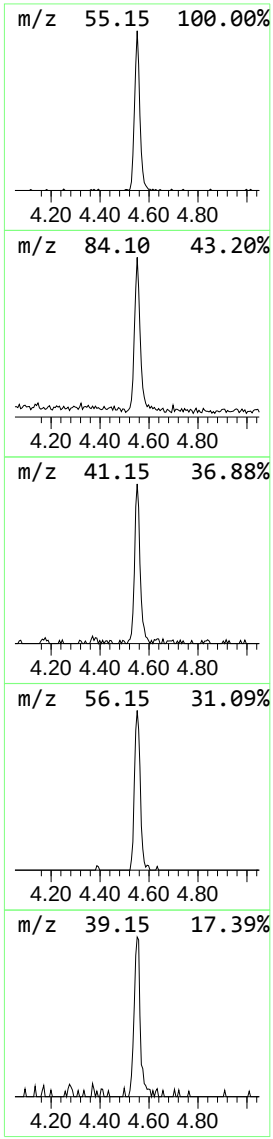
****

Peak Number 1 Cyclopentanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.551	12.54 ng	116242	1,4-Dichlorobenzene-d4	8.105

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanone	84	C5H8O	000120-92-3	91
2	1H-Tetrazole, 1-methyl-	84	C2H4N4	016681-77-9	59
3	2H-Pyran, 3,4-dihydro-	84	C5H8O	000110-87-2	50
4	2(3H)-Furanone	84	C4H4O2	020825-71-2	47
5	2-Hexene	84	C6H12	000592-43-8	45





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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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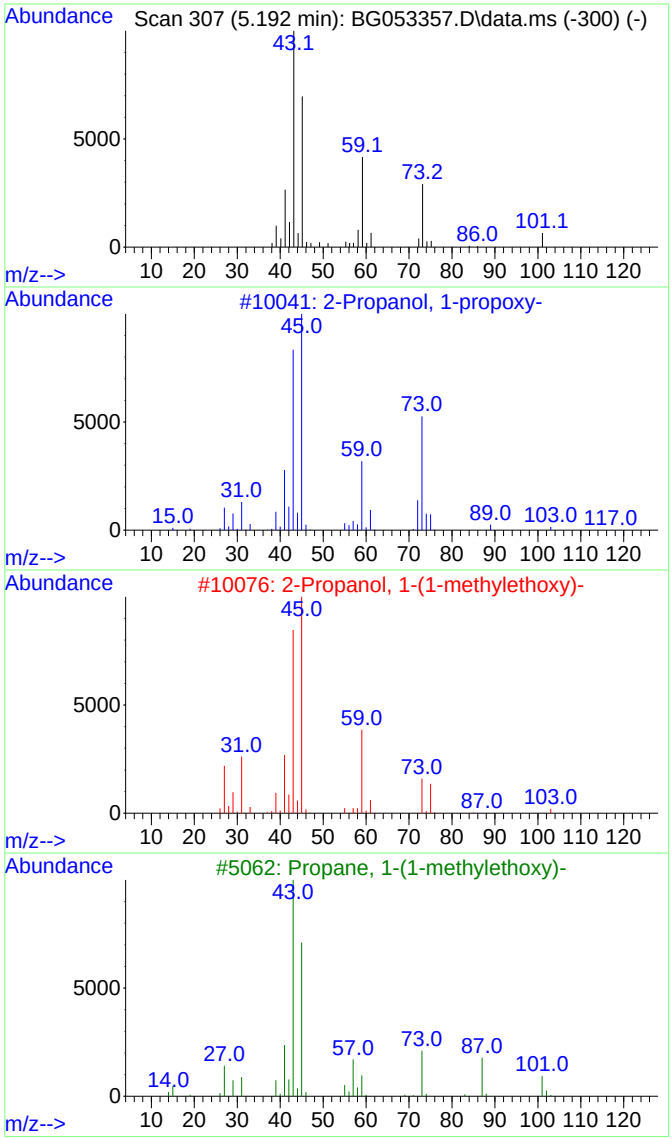
TIC Integration Parameters: LSCINT.P

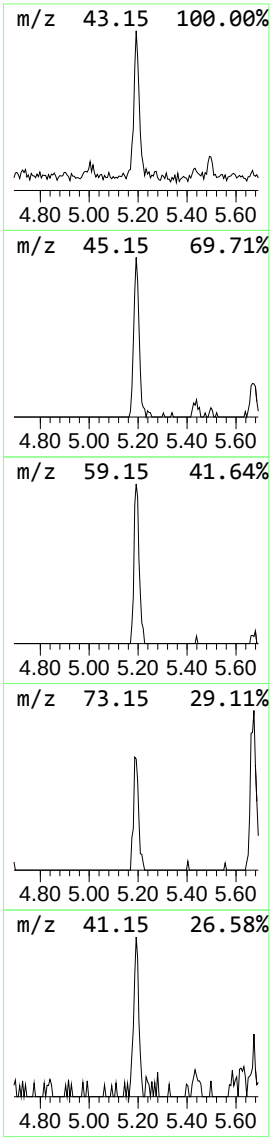
****

Peak Number 2 2-Propanol, 1-propoxy- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.192	5.10 ng	47294	1,4-Dichlorobenzene-d4	8.105

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-propoxy-	118	C6H14O2	001569-01-3	50
2	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45
3	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	40
4	Ethanol, 2-(1-methylethoxy)-	104	C5H12O2	000109-59-1	40
5	Diacetamide	101	C4H7NO2	000625-77-4	38





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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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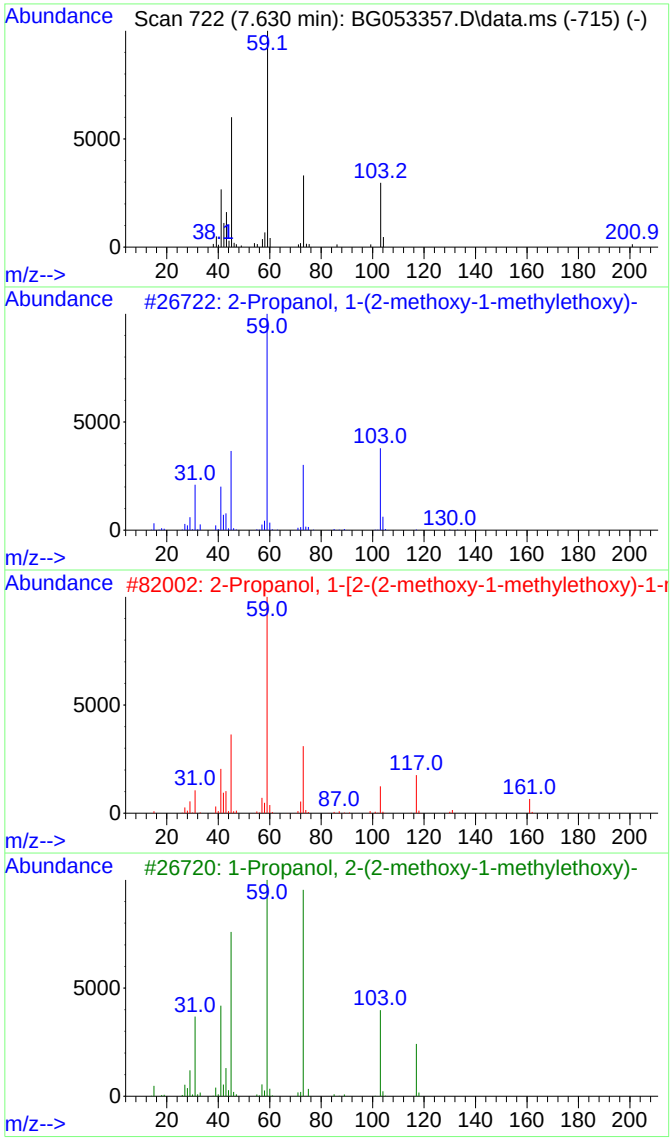
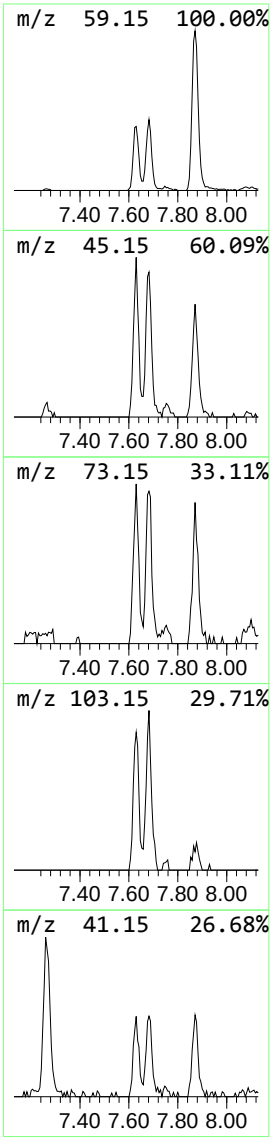
****
Peak Number 3 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.630	6.91 ng	64067	1,4-Dichlorobenzene-d4	8.105

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	72
2	2-Propanol, 1-[2-(2-methoxy-1-me...	206	C10H22O4	020324-33-8	72
3	1-Propanol, 2-(2-methoxy-1-methy...	148	C7H16O3	055956-21-3	59
4	Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	59
5	Ethyl 2,5,8,11,14,17,20-heptaoxa...	382	C17H34O9	1000366-80-5	56





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BNA_G
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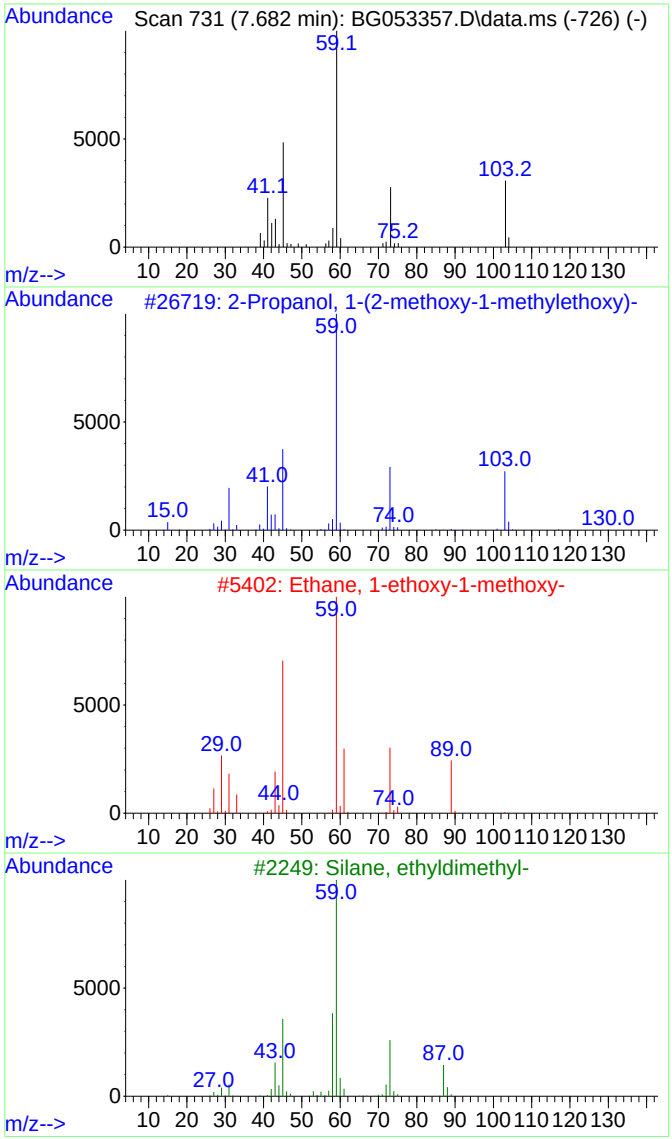
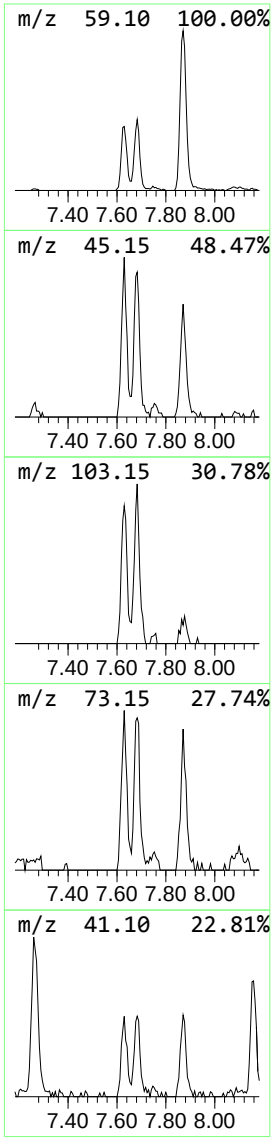
****

Peak Number 4 Ethane, 1-ethoxy-1-methoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.682	6.96 ng	64491	1,4-Dichlorobenzene-d4	8.105

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	83
2	Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	59
3	Silane, ethyldimethyl-	88	C4H12Si	000758-21-4	45
4	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	42
5	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	42





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Operator : CG/JU
Sample : N2482-10
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-15

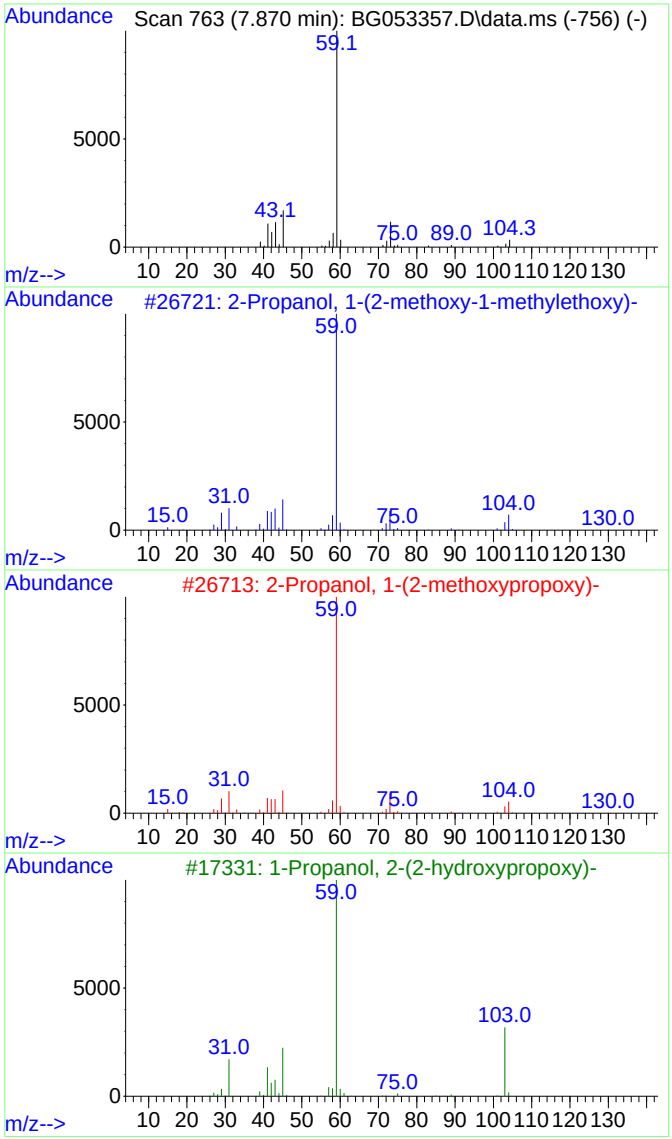
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

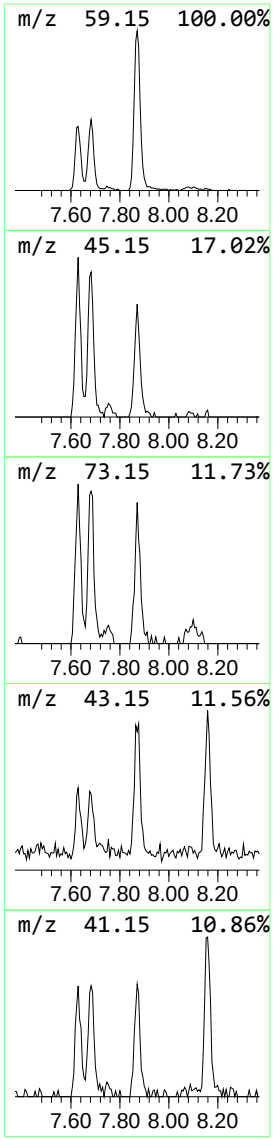
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Propanol, 1-(2-methoxypro... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.870	11.52 ng	106747	1,4-Dichlorobenzene-d4	8.105

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	83
2	2-Propanol, 1-(2-methoxypropoxy)-	148	C7H16O3	013429-07-7	83
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	64
4	1-(1-Methoxypropan-2-yloxy)propa...	190	C9H18O4	1000367-08-6	64
5	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	43





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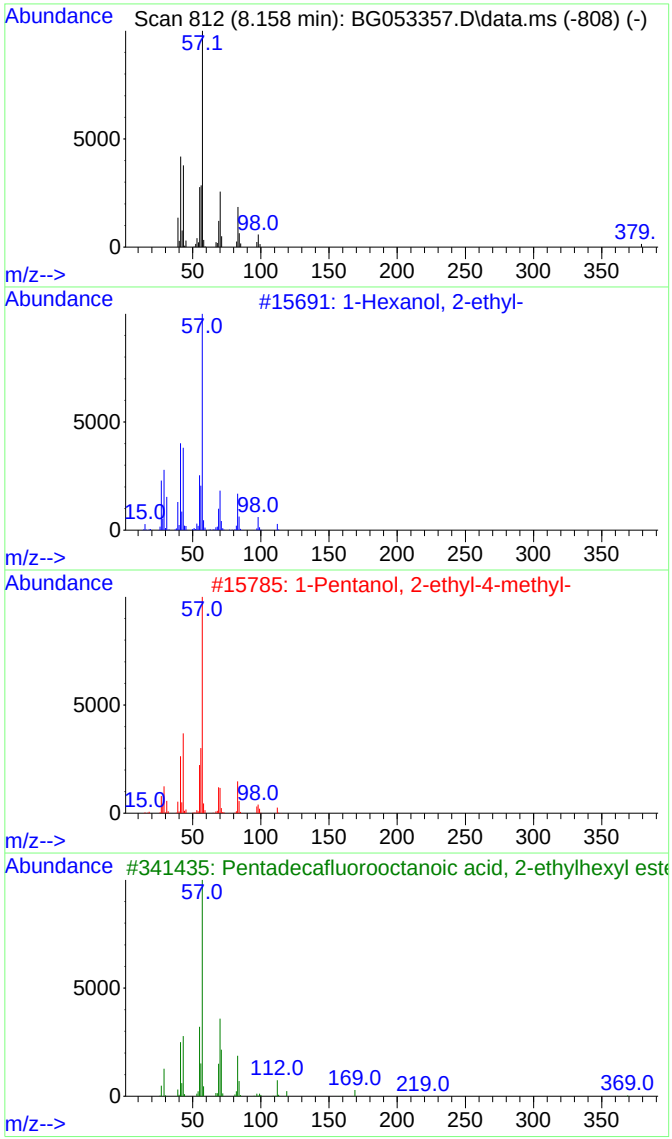
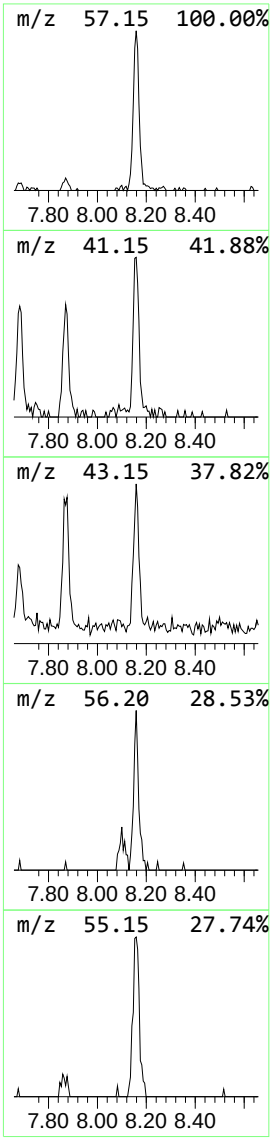
****

Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.158	8.06 ng	74707	1,4-Dichlorobenzene-d4	8.105

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	64
3	Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	64
4	Oxalic acid, bis(2-ethylhexyl) e...	314	C18H34O4	1000309-39-0	53
5	2-Ethyl-1-hexanol, heptafluorobu...	326	C12H17F7O2	1000365-16-0	53





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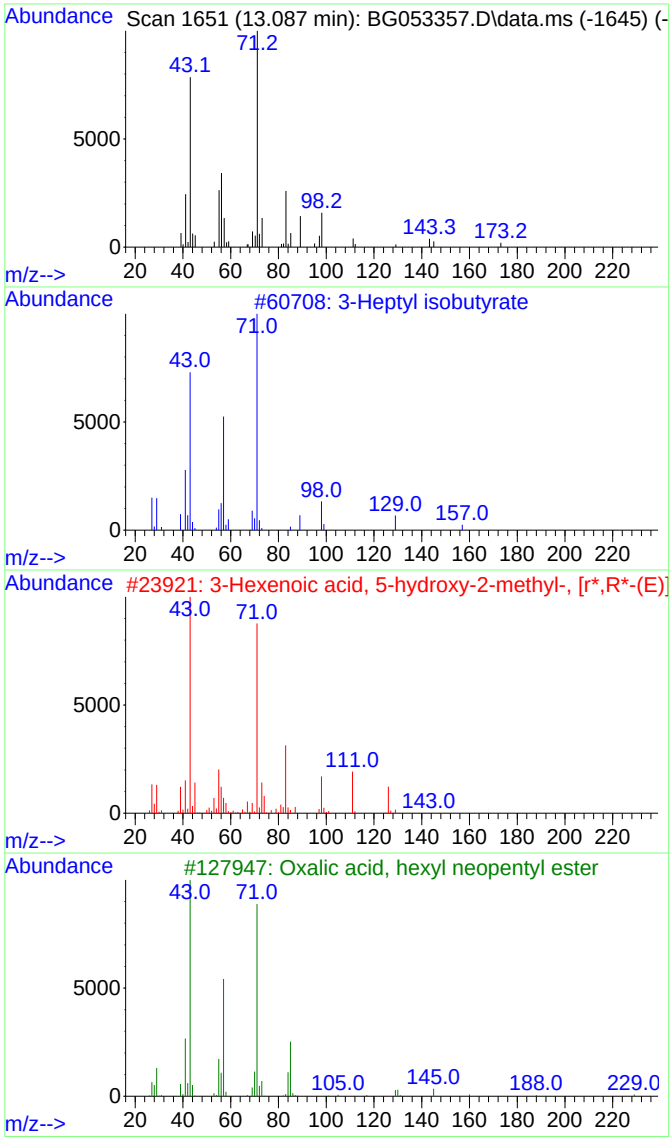
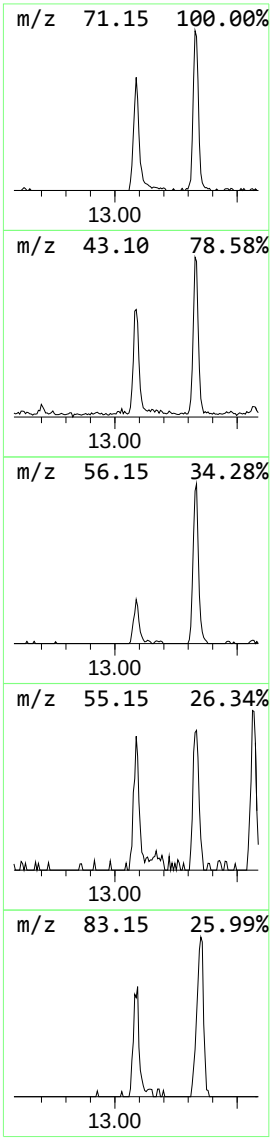
****

Peak Number 7 unknown13.087 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.087	5.26 ng	93179	Acenaphthene-d10	14.726

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Heptyl isobutyrate	186	C11H22O2	1000430-90-3	47
2	3-Hexenoic acid, 5-hydroxy-2-met...	144	C7H12O3	110678-36-9	45
3	Oxalic acid, hexyl neopentyl ester	244	C13H24O4	1000309-73-1	43
4	Butanoic acid, 1-methyloctyl ester	214	C13H26O2	069727-42-0	42
5	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	40





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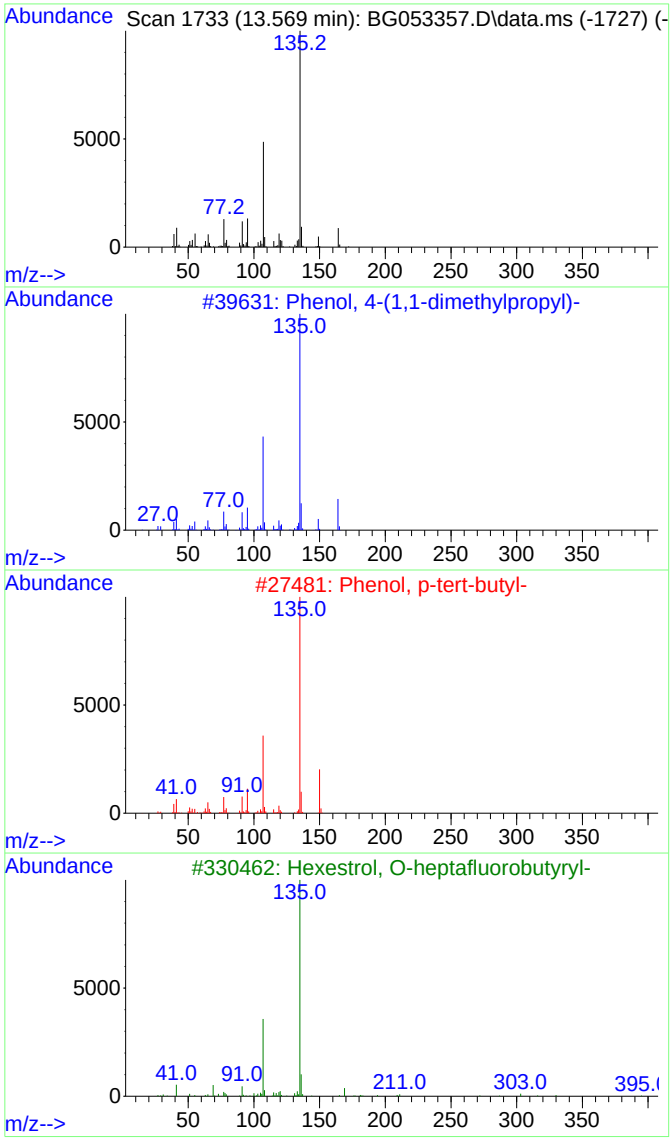
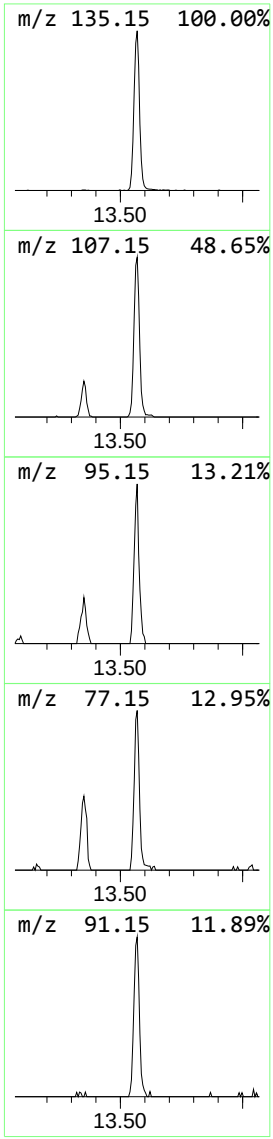
****

Peak Number 8 Phenol, 4-(1,1-dimethylprop... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.569	17.11 ng	303264	Acenaphthene-d10	14.726

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	96
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	78
3	Hexestrol, O-heptafluorobutyryl-	466	C22H21F7O3	1000365-31-9	72
4	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	72
5	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	64





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TIC Library : C:\Database\NIST20.L
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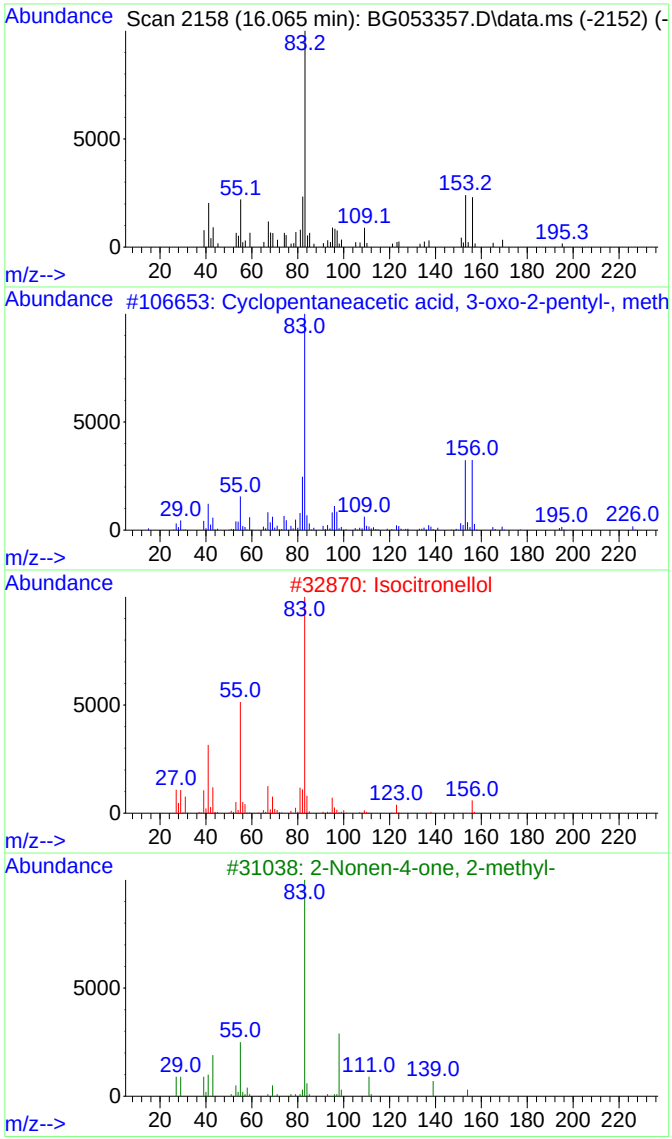
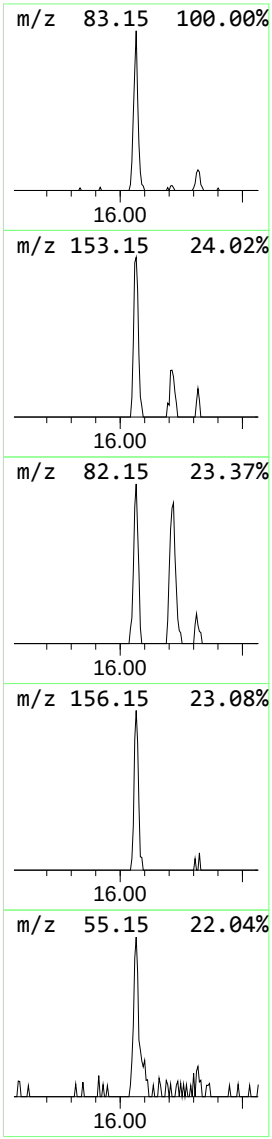
****
Peak Number 9 Cyclopentaneacetic acid, 3-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.065	3.17 ng	56148	Acenaphthene-d10	14.726

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentaneacetic acid, 3-oxo-2...	226	C13H22O3	024851-98-7	83
2	Isocitronellol	156	C10H20O	018479-52-2	45
3	2-Nonen-4-one, 2-methyl-	154	C10H18O	002903-23-3	43
4	Prop-2-ynyl (E)-2-methylbut-2-en...	138	C8H10O2	1000373-72-5	43
5	Ethanone, 1-(1-methylcyclopentyl)-	126	C8H14O	013388-93-7	37





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
Data File : BG053357.D
Acq On : 28 Apr 2022 2:36
Operator : CG/JU
Sample : N2482-10
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-15

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Cyclopentanone	4.551	12.5	ng	116242	1	8.105	185321	20.0
2-Propanol, 1-p...	5.192	5.1	ng	47294	1	8.105	185321	20.0
2-Propanol, 1-(...	7.630	6.9	ng	64067	1	8.105	185321	20.0
Ethane, 1-ethox...	7.682	7.0	ng	64491	1	8.105	185321	20.0
2-Propanol, 1-(...	7.870	11.5	ng	106747	1	8.105	185321	20.0
1-Hexanol, 2-et...	8.158	8.1	ng	74707	1	8.105	185321	20.0
unknown13.087	13.087	5.3	ng	93179	3	14.726	354415	20.0
Phenol, 4-(1,1-...	13.569	17.1	ng	303264	3	14.726	354415	20.0
Cyclopentaneace...	16.065	3.2	ng	56148	3	14.726	354415	20.0