LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052323\
Data File : BG057519.D
Acq On : 23 May 2023 14:34
Operator : CG/JU
Sample : 02867-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP15

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-BG042723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057519.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.973	68	74	83	rBV3	6425	12118	1.27%	0.231%
2	4.407	128	148	157	rBV2	43207	164564	17.21%	3.144%
3	5.147	269	274	285	rBV3	5557	11977	1.25%	0.229%
4	5.388	309	315	321	rBV	13532	20436	2.14%	0.390%
5	5.876	391	398	410	rVB	206730	337831	35.32%	6.453%
6	7.497	667	674	686	rBV	213756	384643	40.22%	7.347%
7	8.355	814	820	827	rBB	67272	113804	11.90%	2.174%
8	9.536	1013	1021	1033	rVB	131228	230978	24.15%	4.412%
9	11.192	1296	1303	1310	rBV	89787	156640	16.38%	2.992%
10	13.348	1665	1670	1674	rVB3	7109	9920	1.04%	0.189%
11	13.595	1705	1712	1719	rBV	387421	560709	58.63%	10.711%
12	14.288	1824	1830	1834	rBV	37918	53527	5.60%	1.022%
13	14.911	1930	1936	1940	rBV	20352	27723	2.90%	0.530%
14	14.969	1940	1946	1959	rVB	144960	229232	23.97%	4.379%
15	16.309	2166	2174	2184	rVB	58488	92597	9.68%	1.769%
16	16.415	2184	2192	2194	rBV2	9367	16259	1.70%	0.311%
17	16.456	2194	2199	2206	rVB	319200	480164	50.20%	9.172%
18	16.873	2264	2270	2277	rVB3	16194	24551	2.57%	0.469%
19	17.713	2406	2413	2420	rBV	209825	318318	33.28%	6.081%
20	18.553	2551	2556	2566	rBV2	30103	56780	5.94%	1.085%
21	20.280	2844	2850	2859	rVB	753891	956421	100.00%	18.270%
22	21.414	3037	3043	3051	rVB	151243	205697	21.51%	3.929%
23	21.572	3066	3070	3080	rBV4	23943	49267	5.15%	0.941%
24	22.019	3139	3146	3153	rBV2	212112	367347	38.41%	7.017%
25	25.514	3731	3741	3755	rVB	117454	353538	36.96%	6.753%

Sum of corrected areas: 5235041

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Misc :
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Instrument :
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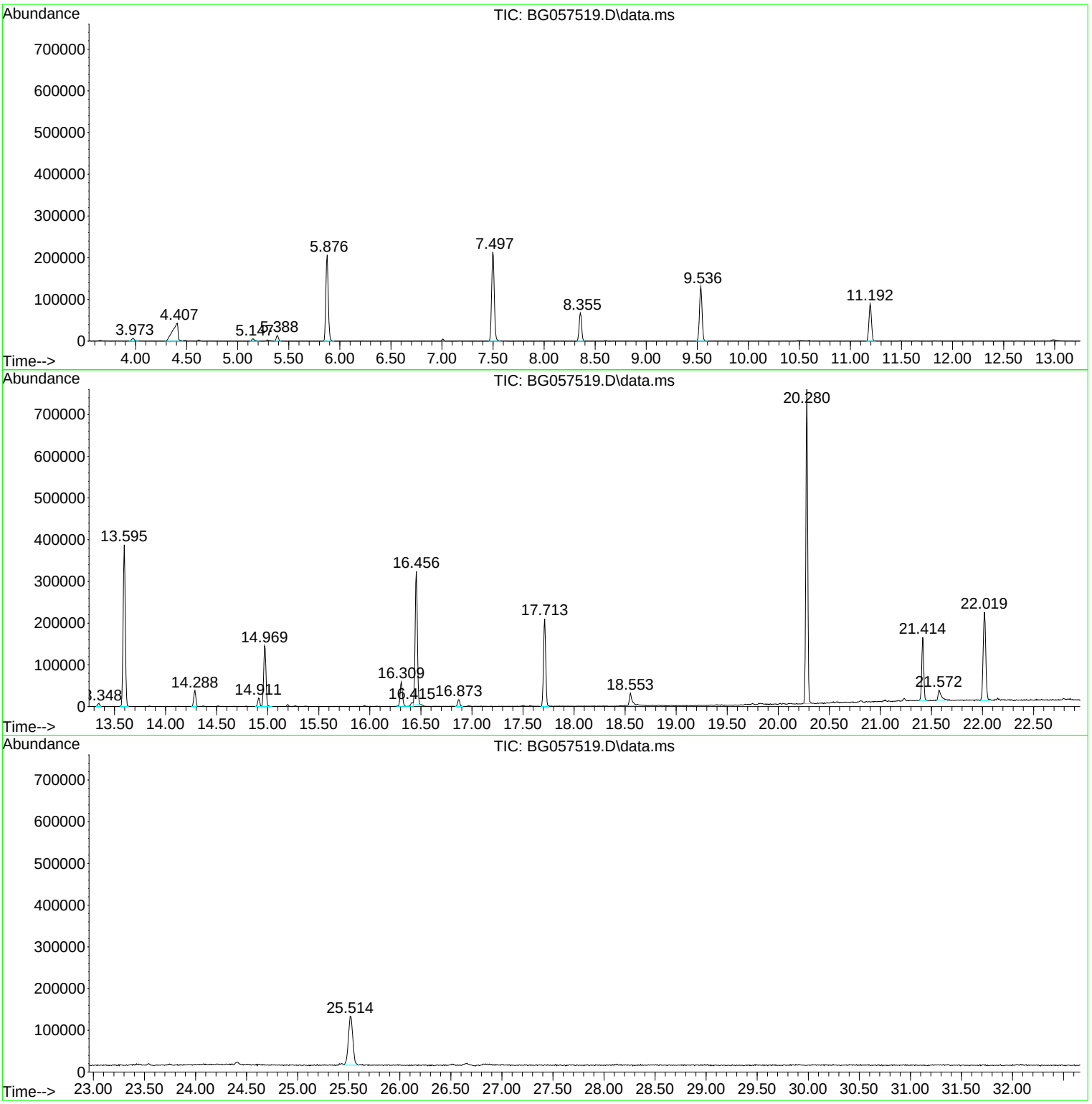
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BG057519.D
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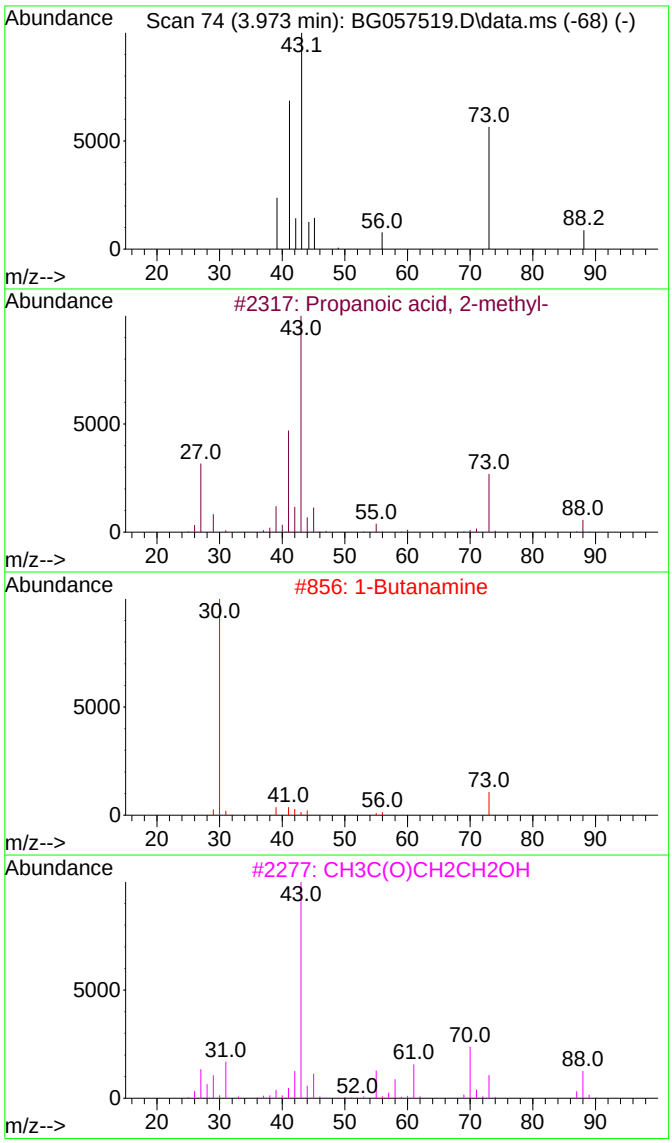
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

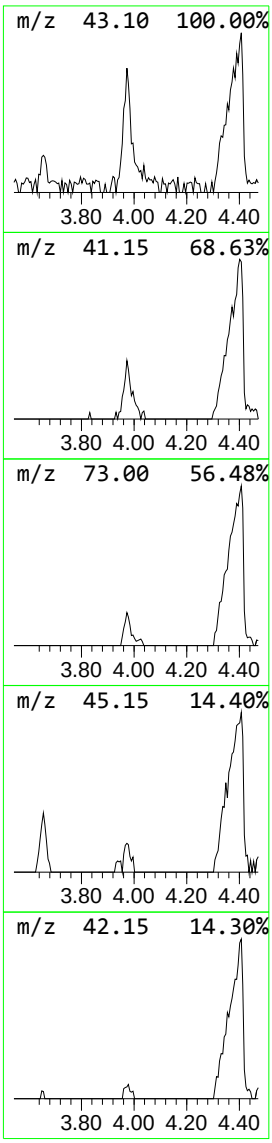
****

Peak Number 1 Propanoic acid, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.973	2.13 ng	12118	1,4-Dichlorobenzene-d4	8.355

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	83
2	1-Butanamine	73	C4H11N	000109-73-9	9
3	CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	9
4	1-Hepten-4-ol	114	C7H14O	003521-91-3	9
5	Guanidine, methyl-	73	C2H7N3	000471-29-4	7





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
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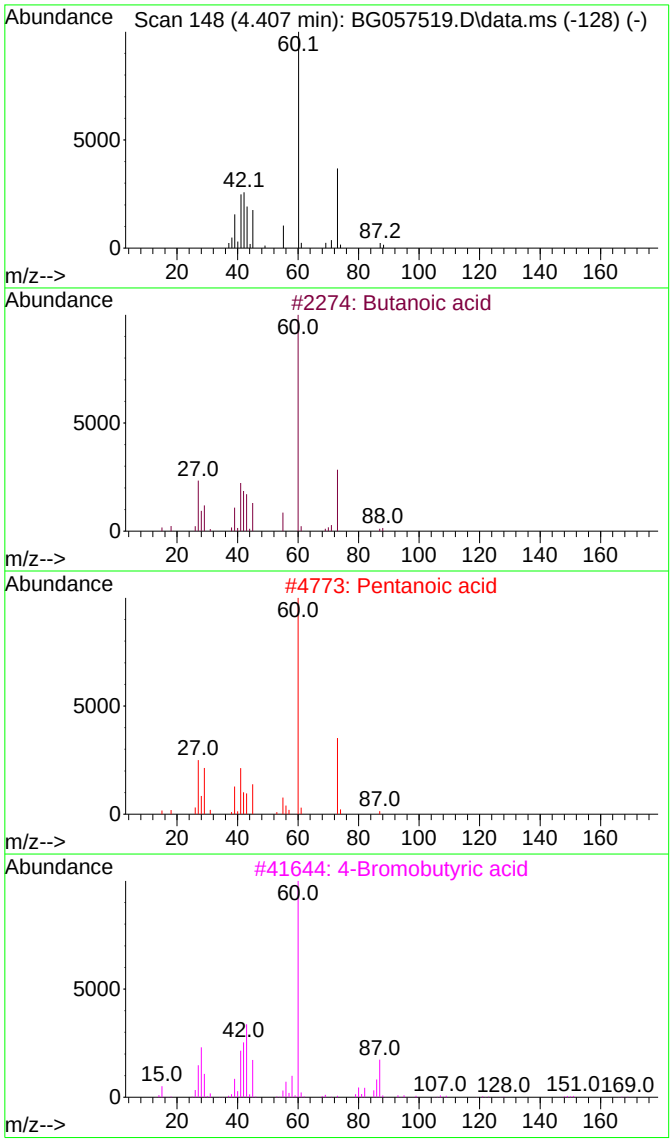
TIC Integration Parameters: LSCINT.P

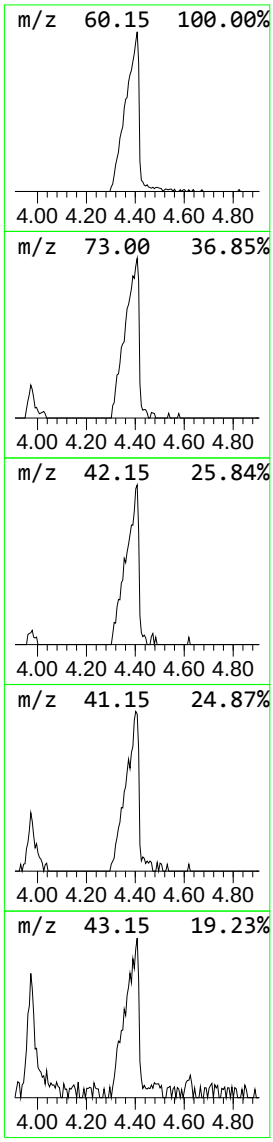
****

Peak Number 2 Butanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.407	28.92 ng	164564	1,4-Dichlorobenzene-d4	8.355

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid	88	C4H8O2	000107-92-6	91
2	Pentanoic acid	102	C5H10O2	000109-52-4	39
3	4-Bromobutyric acid	166	C4H7BrO2	002623-87-2	9
4	Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	9
5	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	9





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Misc :
ALS Vial : 9 Sample Multiplier: 1

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ClientSampleId :
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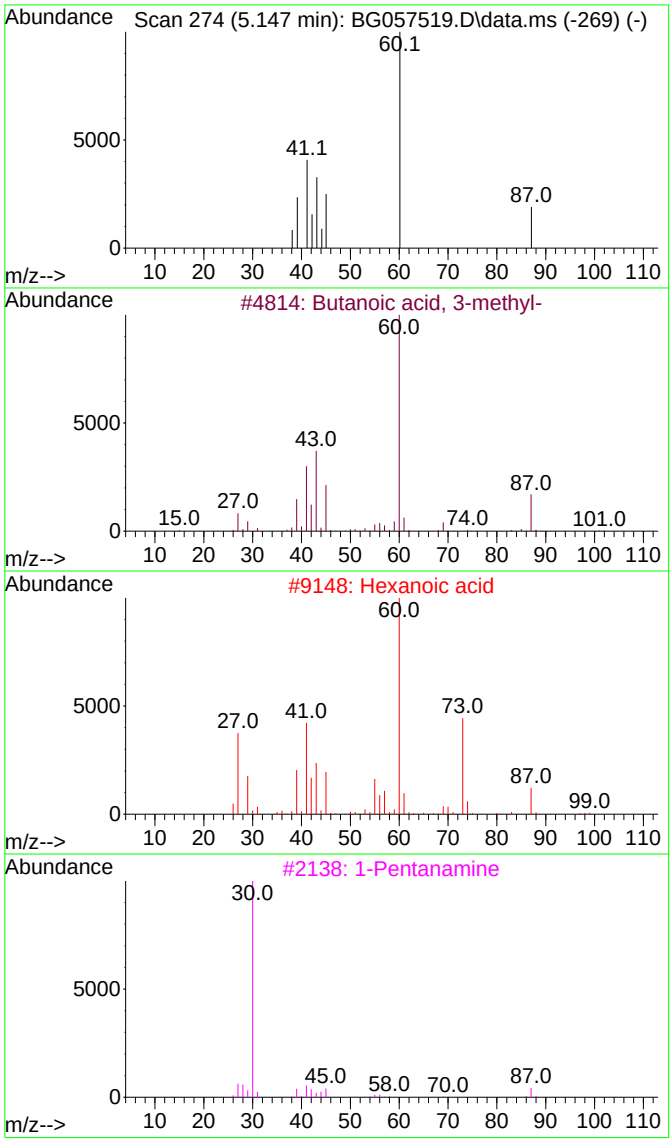
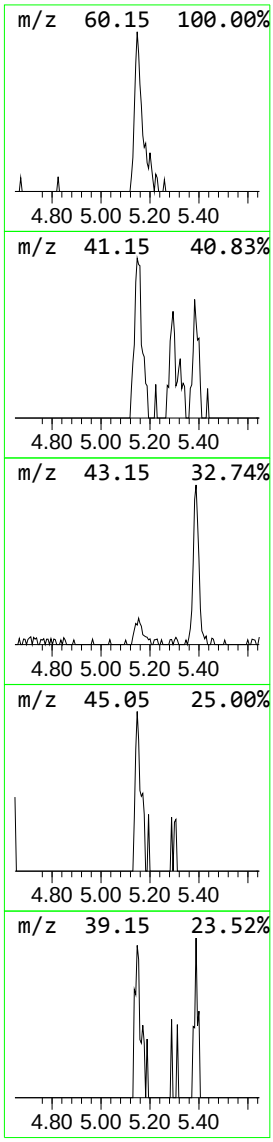
Peak Number 3 unknown5.147 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.147	2.10 ng	11977	1,4-Dichlorobenzene-d4	8.355

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	43
2	Hexanoic acid	116	C6H12O2	000142-62-1	9
3	1-Pentanamine	87	C5H13N	000110-58-7	7
4	Formic acid hydrazide	60	CH4N2O	000624-84-0	7
5	Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	4





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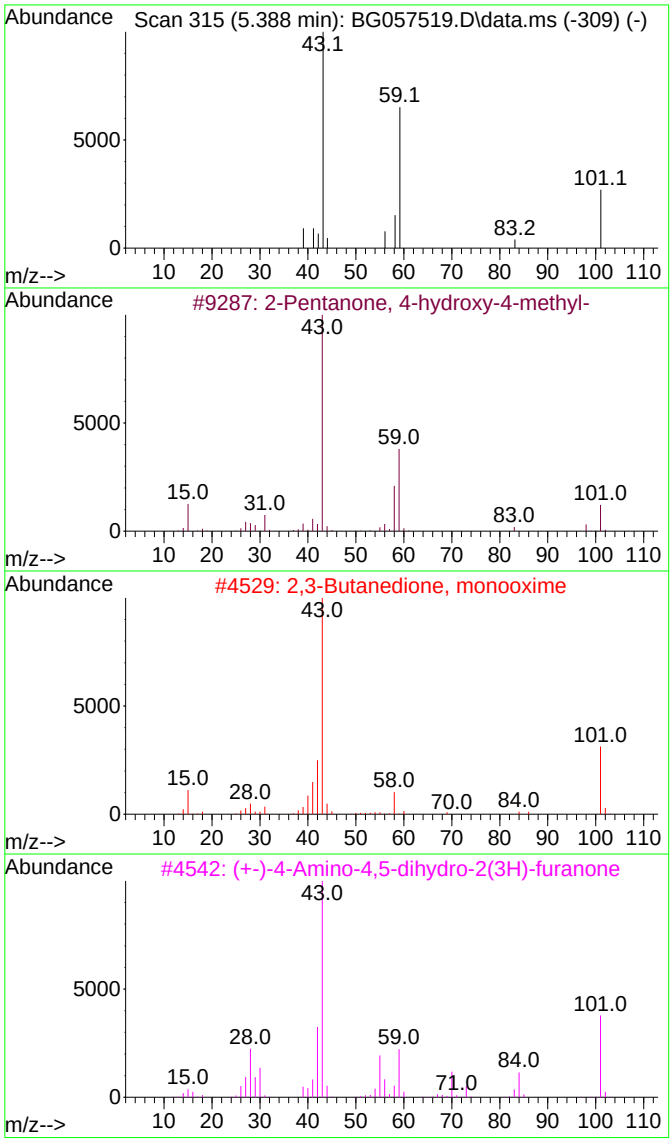
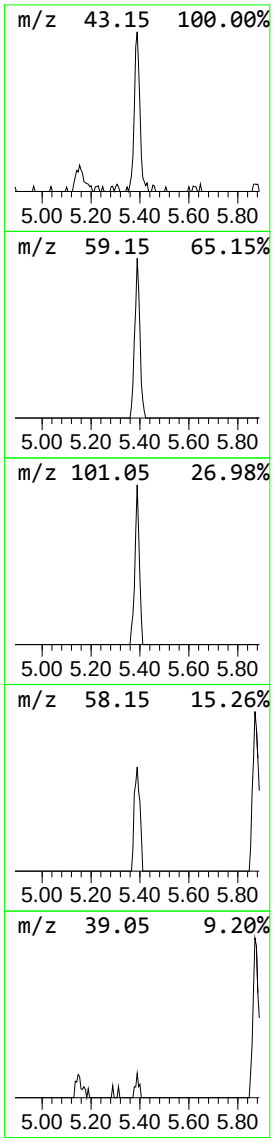
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.388	3.59 ng	20436	1,4-Dichlorobenzene-d4	8.355

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	78
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4	Diacetamide	101	C4H7NO2	000625-77-4	5
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	5





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ALS Vial : 9 Sample Multiplier: 1

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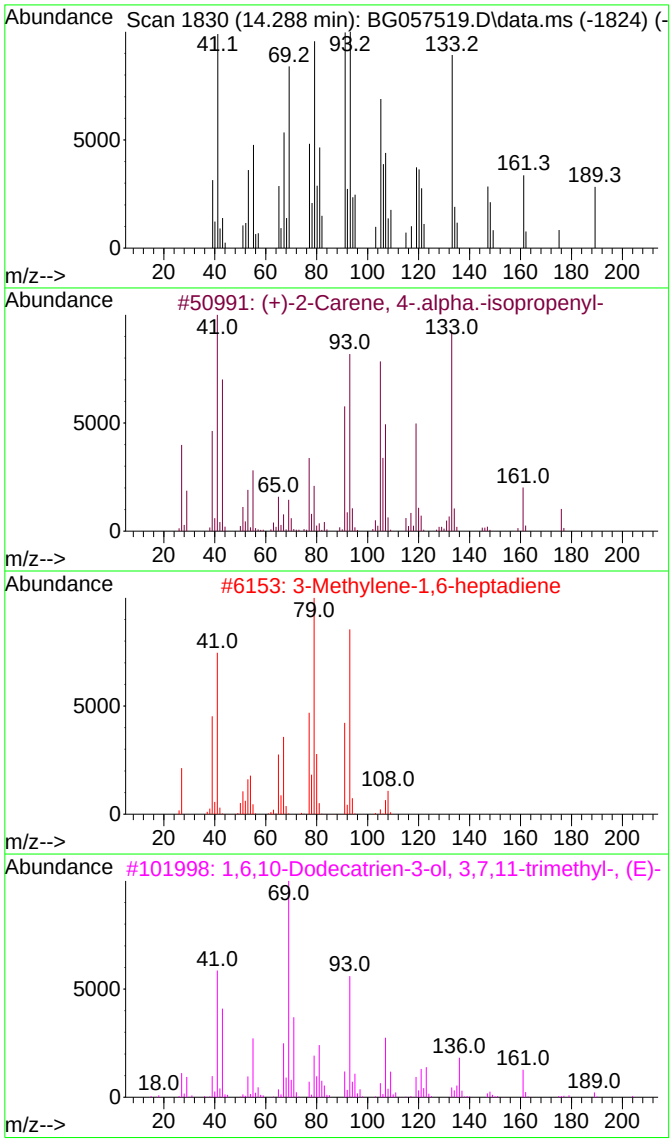
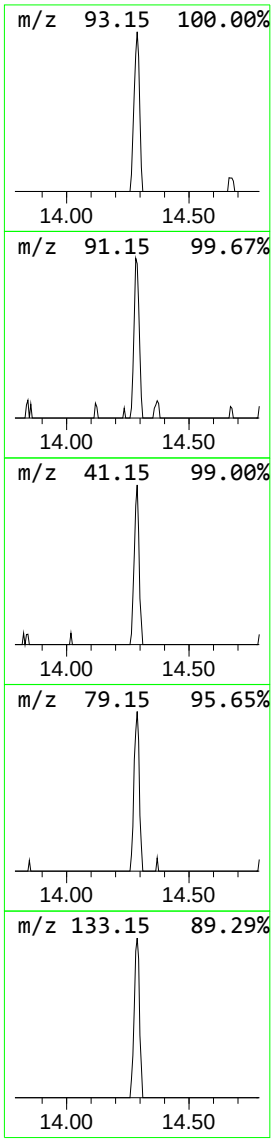
****

Peak Number 5 unknown14.288 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.288	4.67 ng	53527	Acenaphthene-d10	14.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-2-Carene, 4-.alpha.-isoprope...	176	C13H20	1000151-26-0	38
2	3-Methylene-1,6-heptadiene	108	C8H12	016626-48-5	38
3	1,6,10-Dodecatrien-3-ol, 3,7,11-...	222	C15H26O	040716-66-3	35
4	Cyclohexane, 1,5-diethenyl-3-met...	162	C12H18	074742-35-1	35
5	Bicyclo[4.1.0]heptane, 7-methylene-	108	C8H12	054211-14-2	22





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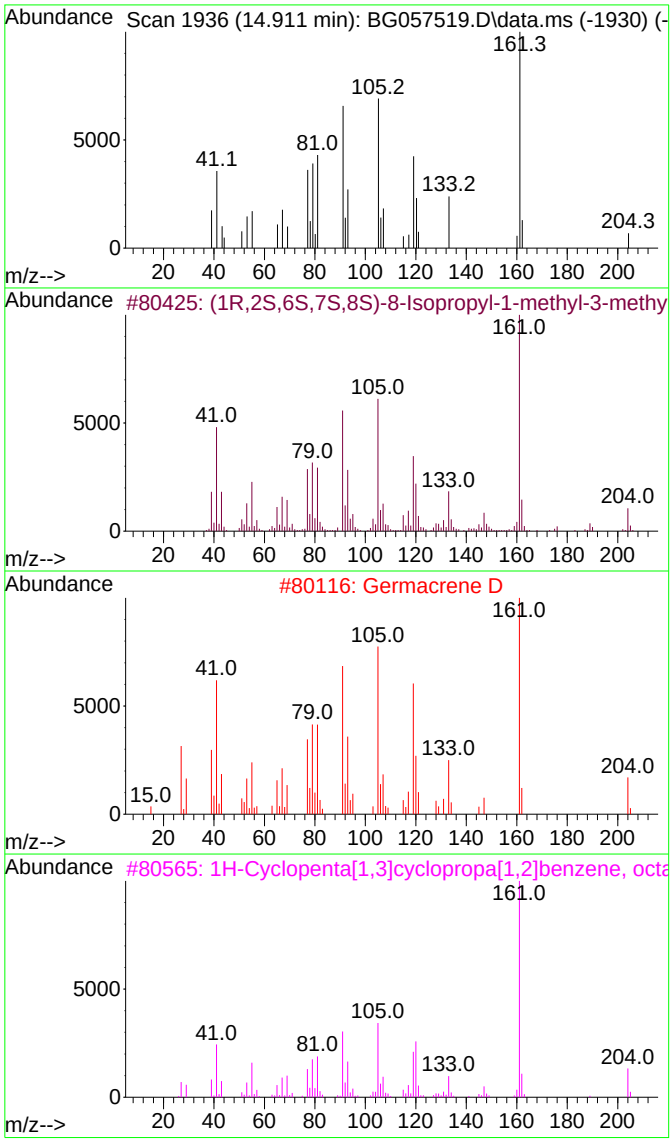
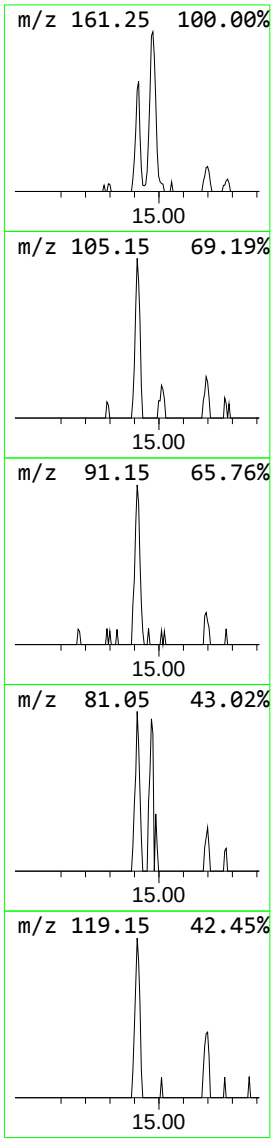
****

Peak Number 6 (1R,2S,6S,7S,8S)-8-Isopropy... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.911	2.42 ng	27723	Acenaphthene-d10	14.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1R,2S,6S,7S,8S)-8-Isopropyl-1-m...	204	C15H24	018252-44-3	94
2	Germacrene D	204	C15H24	023986-74-5	72
3	1H-Cyclopenta[1,3]cyclopropa[1,2...	204	C15H24	013744-15-5	50
4	6,7-Dimethyl-1,2,3,5,8,8a-hexahy...	162	C12H18	107914-92-1	50
5	Tetracyclo[6.1.0.0(2,4).0(5,7)]n...	204	C15H24	051898-92-1	49





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TIC Library : C:\Database\NIST20.L
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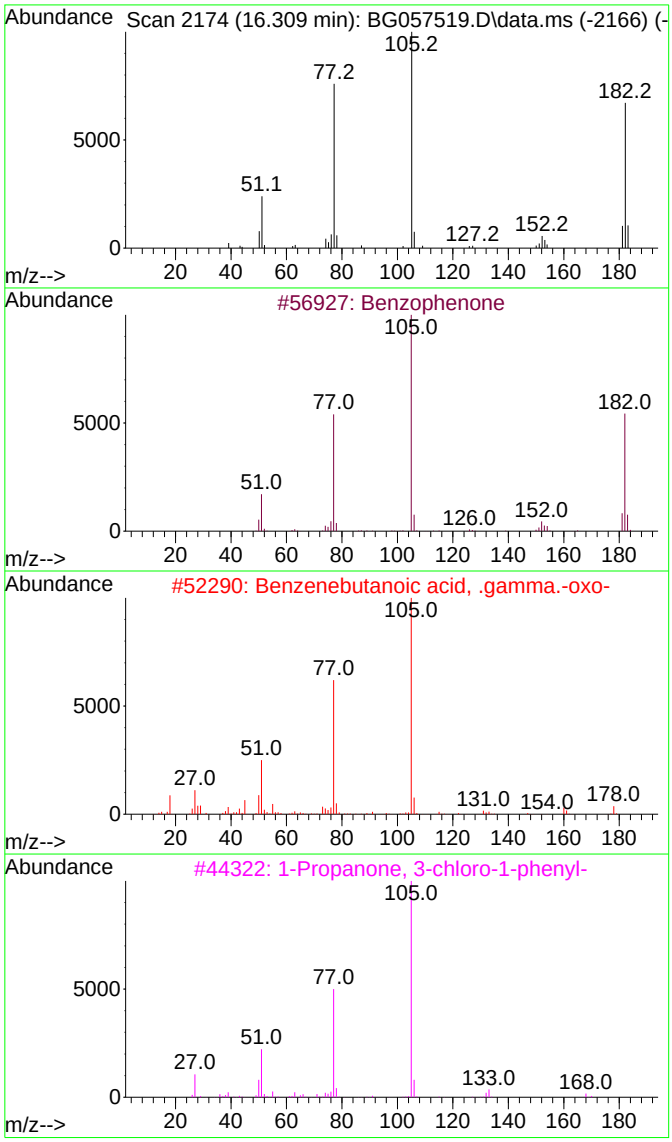
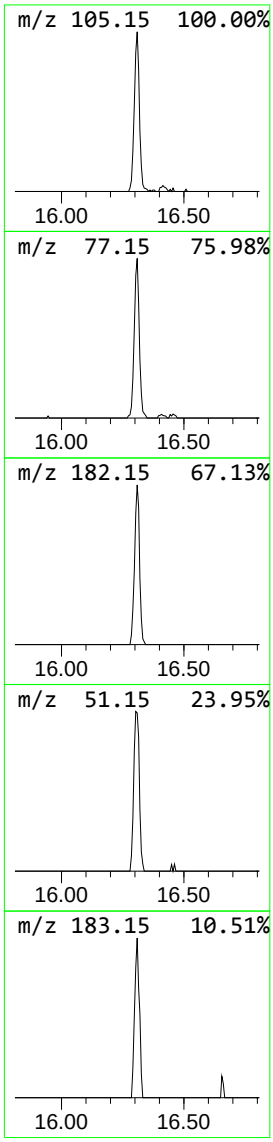
Peak Number 7 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.309	8.08 ng	92597	Acenaphthene-d10	14.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	50
3	1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	50
4	2-Phenyl-4-ethylidene-2-oxazolin...	187	C11H9NO2	037791-41-6	50
5	Benzene, (trimethoxymethyl)-	182	C10H14O3	000707-07-3	50





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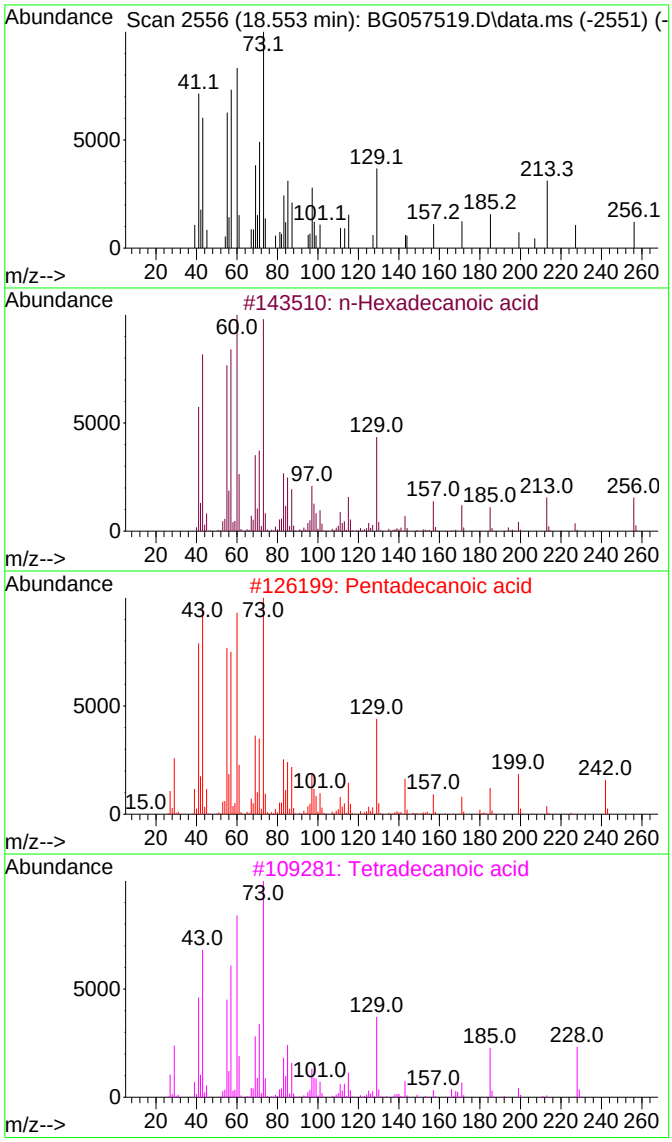
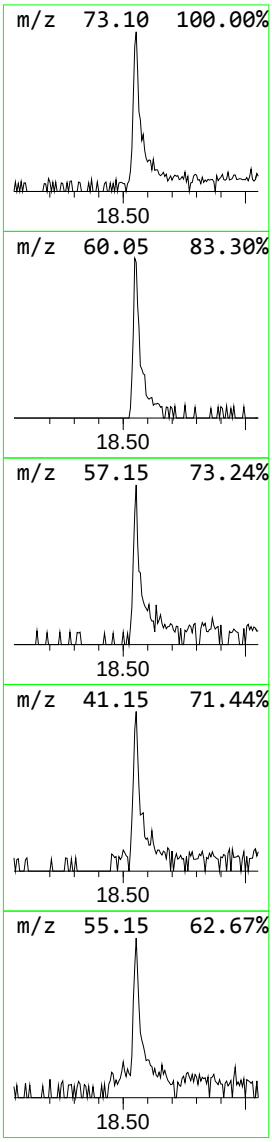
Peak Number 8 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.553	3.57 ng	56780	Phenanthrene-d10	17.713

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	62
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	50
4	Dodecanoic acid	200	C12H24O2	000143-07-7	47
5	Tridecanoic acid	214	C13H26O2	000638-53-9	47





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TIC Library : C:\Database\NIST20.L
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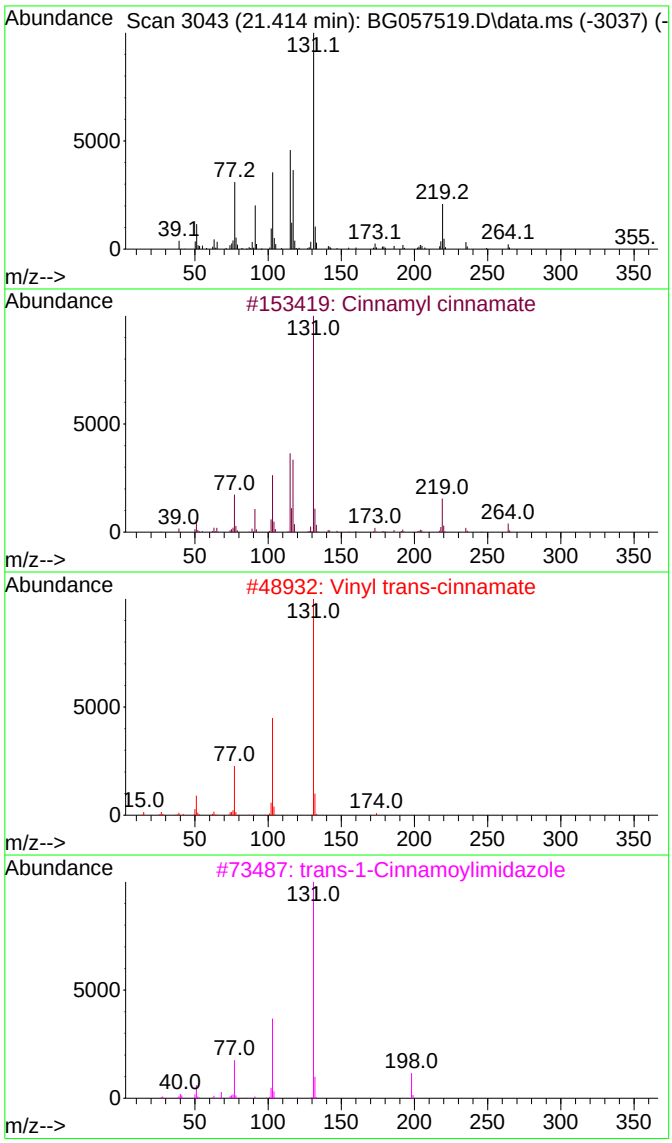
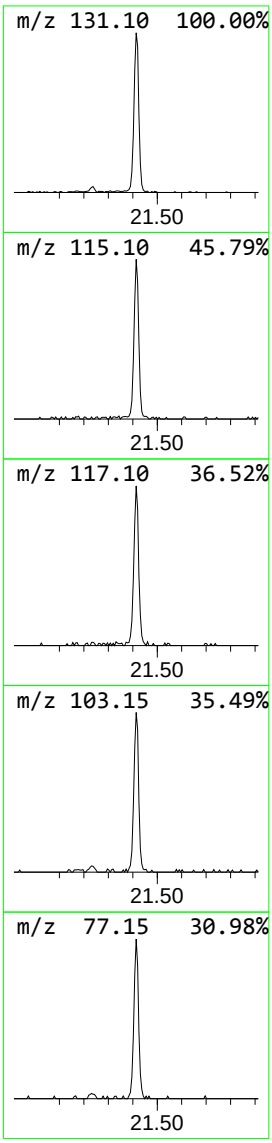
Peak Number 9 Cinnamyl cinnamate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.414	11.20 ng	205697	Chrysene-d12	22.019

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91
2	Vinyl trans-cinnamate	174	C11H10O2	017719-70-9	49
3	trans-1-Cinnamoylimidazole	198	C12H10N2O	001138-15-4	47
4	(2E)-N-(2-Fluorophenyl)-3-phenyl...	241	C15H12FNO	025893-50-9	47
5	N-(p-Vinylbenzoyl)-l-alanine	219	C12H13NO3	139184-60-4	47





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ALS Vial : 9 Sample Multiplier: 1

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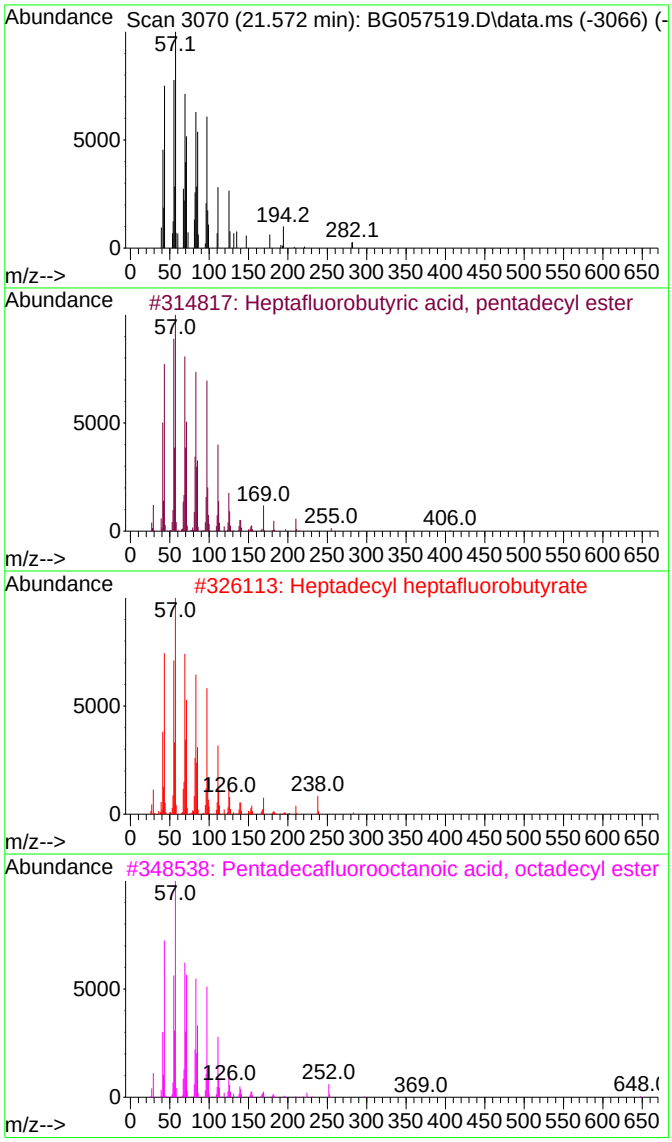
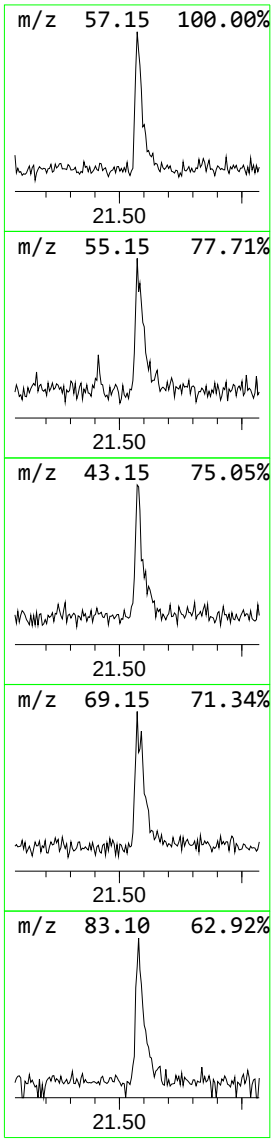
****
Peak Number 10 Heptafluorobutyric acid, pe... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.572	2.68 ng	49267	Chrysene-d12	22.019

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	81
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	74
3	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	74
4	Hexacosyl trifluoroacetate	478	C28H53F3O2	1000351-75-0	72
5	Hexacosyl heptafluorobutyrate	578	C30H53F7O2	1000351-83-3	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052323\
Data File : BG057519.D
Acq On : 23 May 2023 14:34
Operator : CG/JU
Sample : 02867-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP15

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.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
Propanoic acid,...	3.973	2.1	ng	12118	1	8.355	113804	20.0
Butanoic acid	4.407	28.9	ng	164564	1	8.355	113804	20.0
unknown5.147	5.147	2.1	ng	11977	1	8.355	113804	20.0
2-Pentanone, 4-...	5.388	3.6	ng	20436	1	8.355	113804	20.0
unknown14.288	14.288	4.7	ng	53527	3	14.969	229232	20.0
(1R,2S,6S,7S,8S...	14.911	2.4	ng	27723	3	14.969	229232	20.0
Benzophenone	16.309	8.1	ng	92597	3	14.969	229232	20.0
n-Hexadecanoic ...	18.553	3.6	ng	56780	4	17.713	318318	20.0
Cinnamyl cinnamate	21.414	11.2	ng	205697	5	22.019	367347	20.0
Heptafluorobuty...	21.572	2.7	ng	49267	5	22.019	367347	20.0