LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051324\
Data File : BG061177.D
Acq On : 13 May 2024 16:05
Operator : MA/JU
Sample : P2449-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1011UMR-RB240508-01

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-BG043024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG061177.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.073	8	14	21	rBV3	25970	53285	1.95%	0.461%
2	3.149	21	27	42	rVB	902325	1436836	52.52%	12.425%
3	5.523	425	431	440	rVB	220404	341000	12.46%	2.949%
4	7.103	694	700	709	rVB	124863	217701	7.96%	1.882%
5	7.926	834	840	846	rBV	90799	146821	5.37%	1.270%
6	7.990	846	851	856	rVB2	26576	40879	1.49%	0.353%
7	9.019	1021	1026	1030	rBV2	24218	37269	1.36%	0.322%
8	9.083	1030	1037	1049	rVB	313156	545807	19.95%	4.720%
9	10.722	1309	1316	1323	rBV	98148	168968	6.18%	1.461%
10	12.538	1618	1625	1630	rBV	28918	40734	1.49%	0.352%
11	12.914	1684	1689	1697	rBV2	31686	50077	1.83%	0.433%
12	13.178	1724	1734	1741	rBV	814914	1310827	47.92%	11.335%
13	14.559	1959	1969	1977	rBV	168541	265902	9.72%	2.299%
14	15.376	2099	2108	2114	rBV3	29811	51909	1.90%	0.449%
15	16.051	2216	2223	2235	rBV	820322	1290926	47.19%	11.163%
16	17.303	2430	2436	2444	rBV	256749	389753	14.25%	3.370%
17	17.973	2545	2550	2555	rBV2	58543	72167	2.64%	0.624%
18	18.496	2633	2639	2644	rVB2	22625	30375	1.11%	0.263%
19	18.713	2671	2676	2681	rBV2	27282	36515	1.33%	0.316%
20	19.929	2876	2883	2892	rVB	1968781	2735720	100.00%	23.656%
21	20.611	2992	2999	3004	rBV2	50932	66225	2.42%	0.573%
22	21.563	3155	3161	3169	rVB2	313600	513475	18.77%	4.440%
23	23.002	3397	3406	3421	rBV	540881	1138967	41.63%	9.849%
24	24.682	3681	3692	3703	rBV	190196	582396	21.29%	5.036%

Sum of corrected areas: 11564534

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051324\
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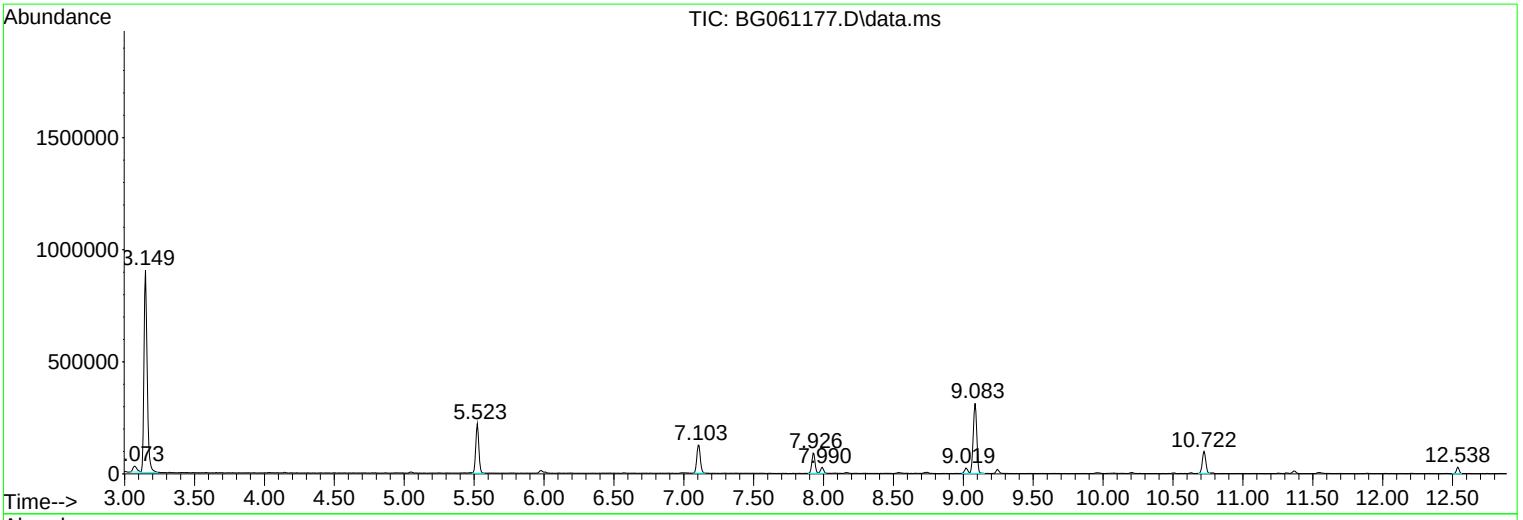
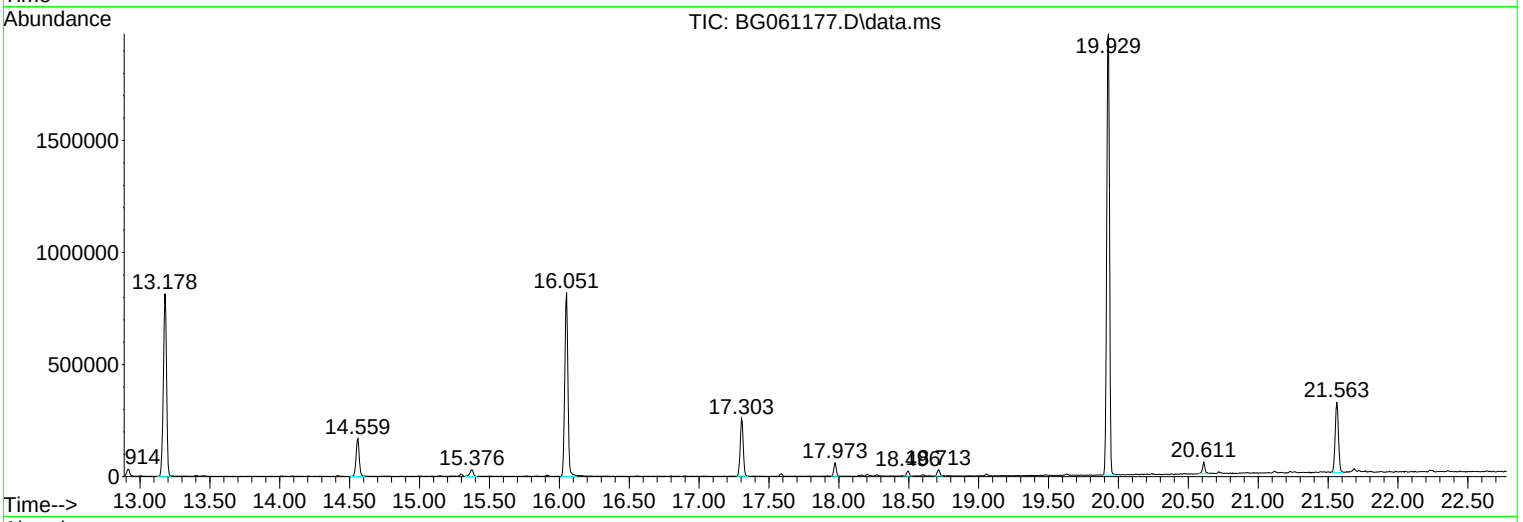
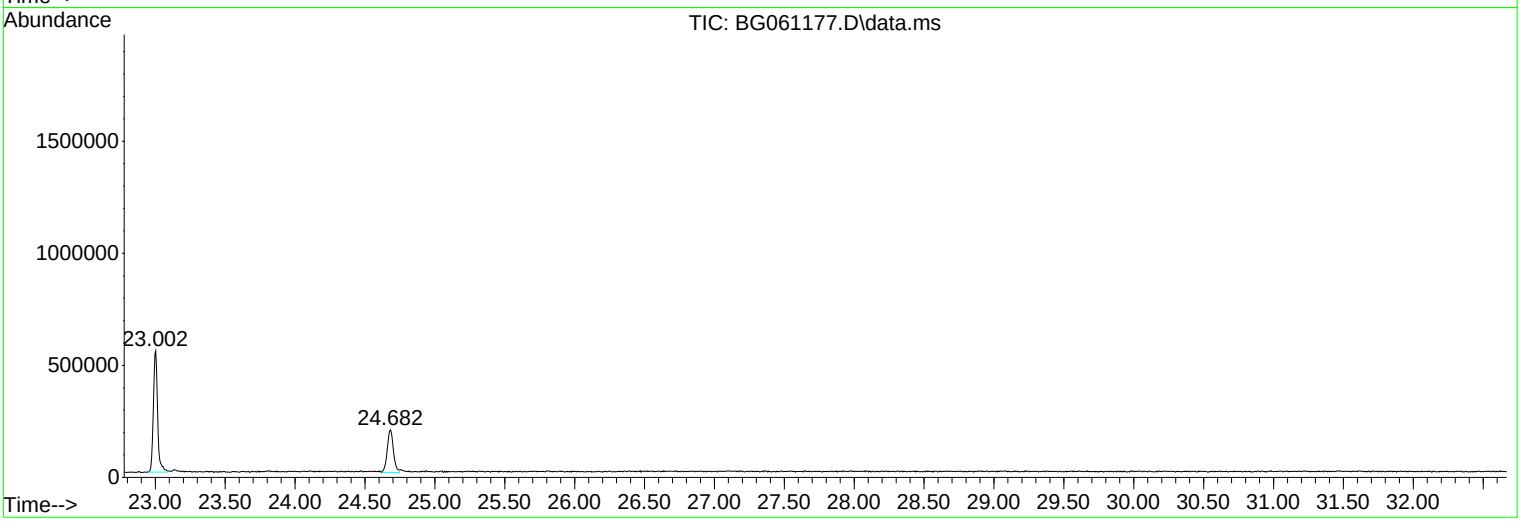
ClientSampleId :
1011UMR-RB240508-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.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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TIC Library : C:\Database\NIST20.L
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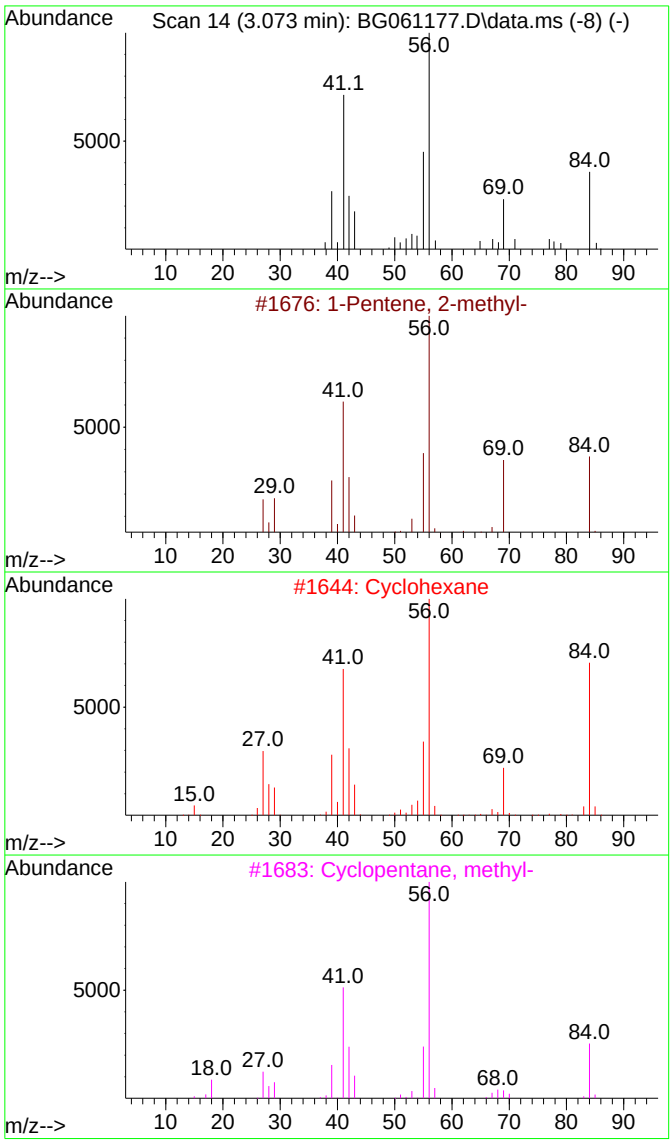
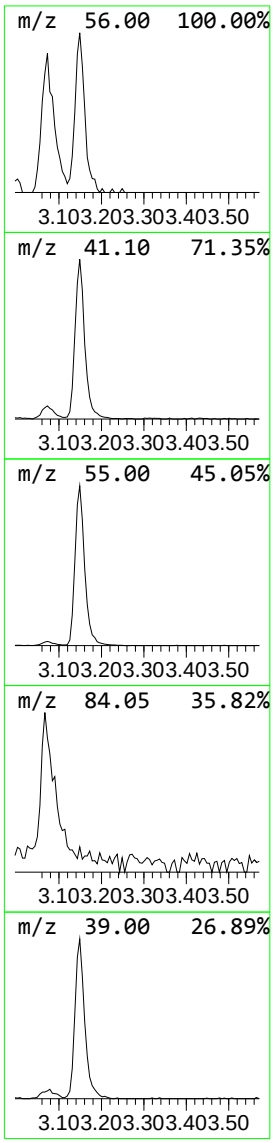
****
Peak Number 1 1-Pentene, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.073	7.26 ng	53285	1,4-Dichlorobenzene-d4	7.926

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	83
2	Cyclohexane	84	C6H12	000110-82-7	80
3	Cyclopentane, methyl-	84	C6H12	000096-37-7	72
4	2-Amino-oxazole	84	C3H4N2O	004570-45-0	72
5	1-Hexene, 3,4-dimethyl-	112	C8H16	016745-94-1	59





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Data File : BG061177.D
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Operator : MA/JU
Sample : P2449-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1011UMR-RB240508-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

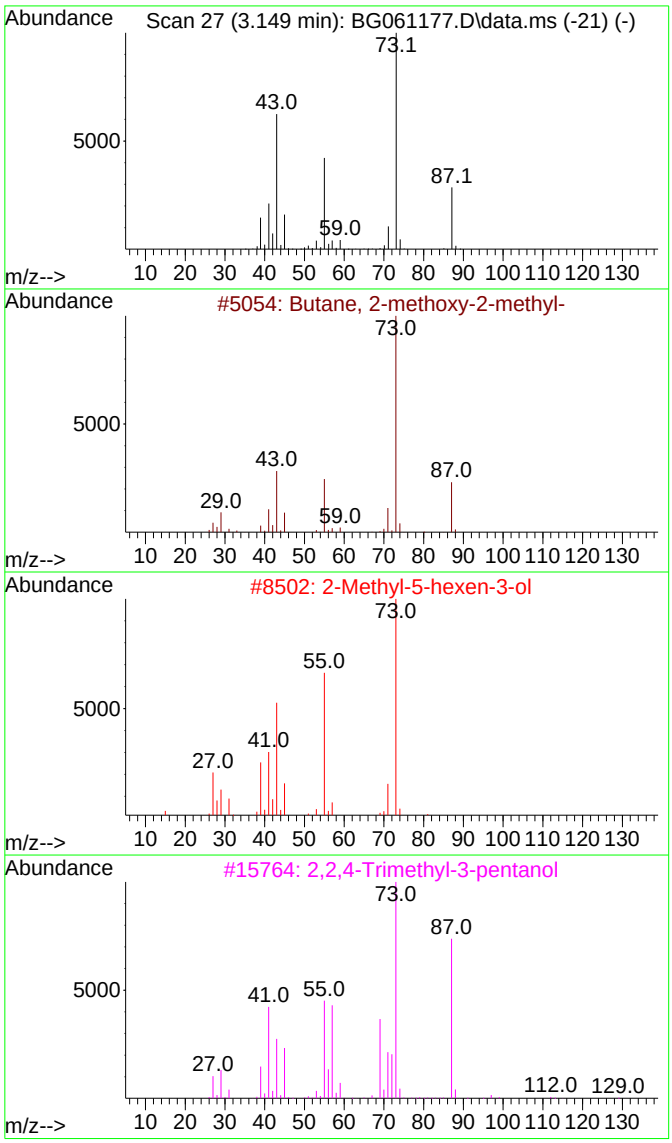
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

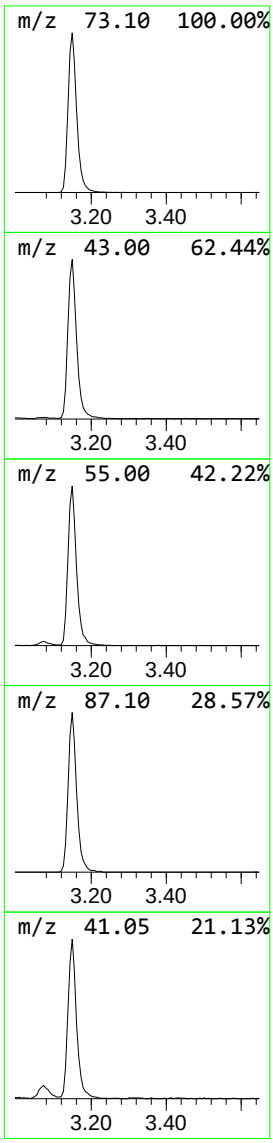
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.149	195.73 ng	1436840	1,4-Dichlorobenzene-d4	7.926

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	90
2	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	47
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	33
4	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	28
5	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051324\
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Acq On : 13 May 2024 16:05
Operator : MA/JU
Sample : P2449-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1011UMR-RB240508-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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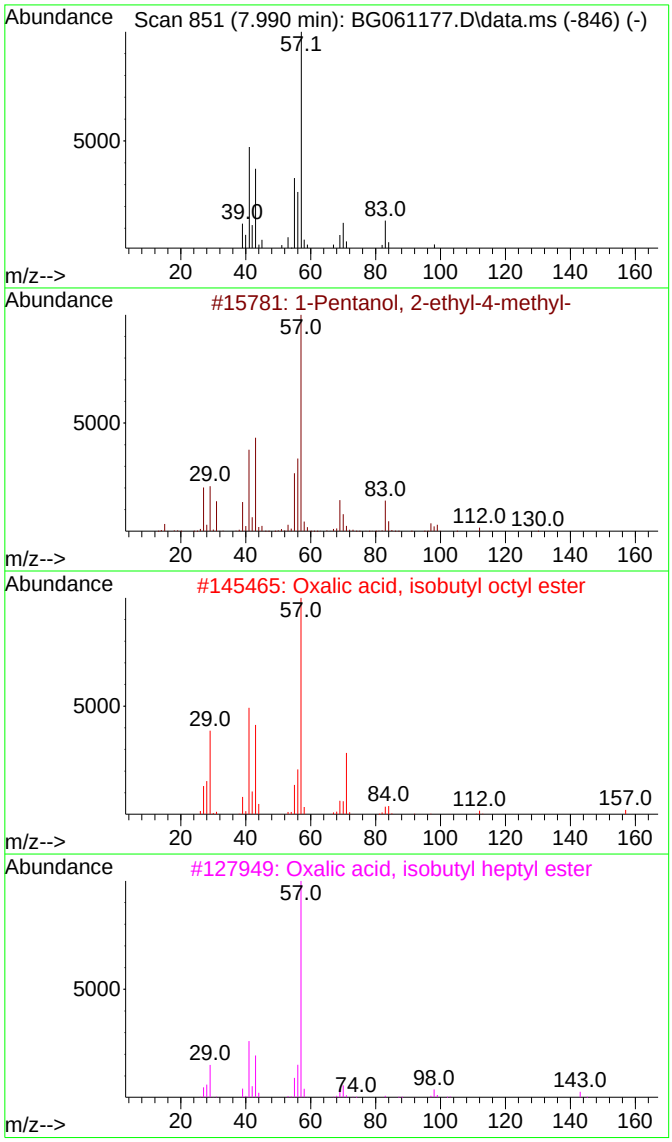
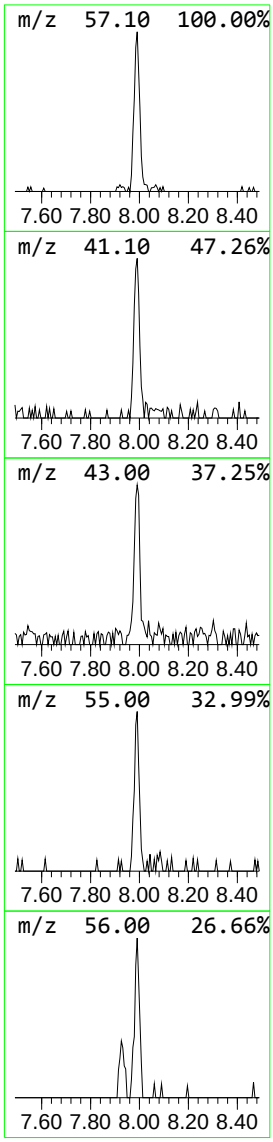
****
Peak Number 3 1-Pentanol, 2-ethyl-4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.990	5.57 ng	40879	1,4-Dichlorobenzene-d4	7.926

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	45
2	Oxalic acid, isobutyl octyl ester	258	C14H26O4	1000309-37-3	38
3	Oxalic acid, isobutyl heptyl ester	244	C13H24O4	1000309-37-2	37
4	Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	37
5	Oxalic acid, heptyl propyl ester	230	C12H22O4	1000309-26-0	37





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Acq On : 13 May 2024 16:05
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Sample : P2449-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1011UMR-RB240508-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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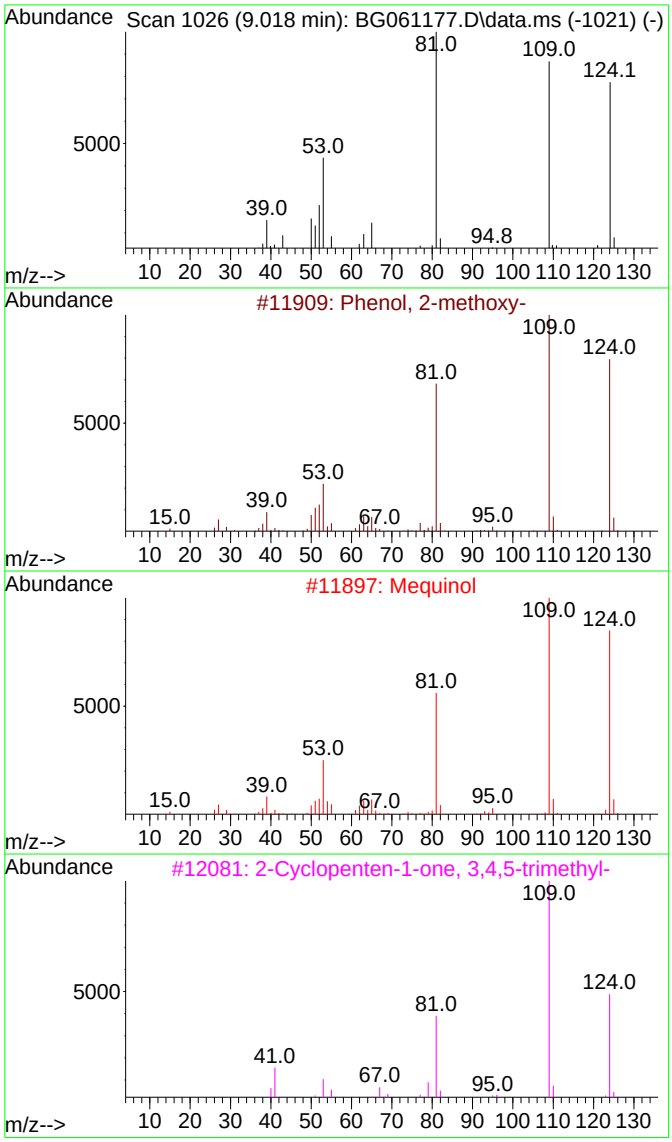
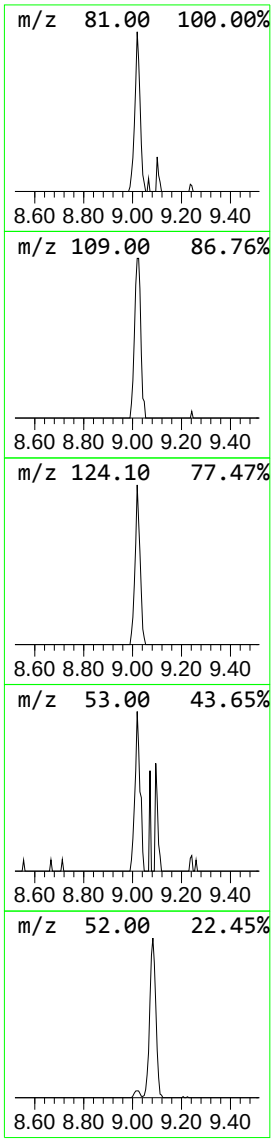
****

Peak Number 4 Phenol, 2-methoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.018	5.08 ng	37269	1,4-Dichlorobenzene-d4	7.926

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	91
2	Mequinol	124	C7H8O2	000150-76-5	64
3	2-Cyclopenten-1-one, 3,4,5-trime...	124	C8H12O	055683-21-1	47
4	Ethanone, 1-(1-cyclohexen-1-yl)-	124	C8H12O	000932-66-1	43
5	Species: cyclopent-3-ene-1,1,2-t...	308	C16H12N4O3	1000277-65-8	42





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Sample : P2449-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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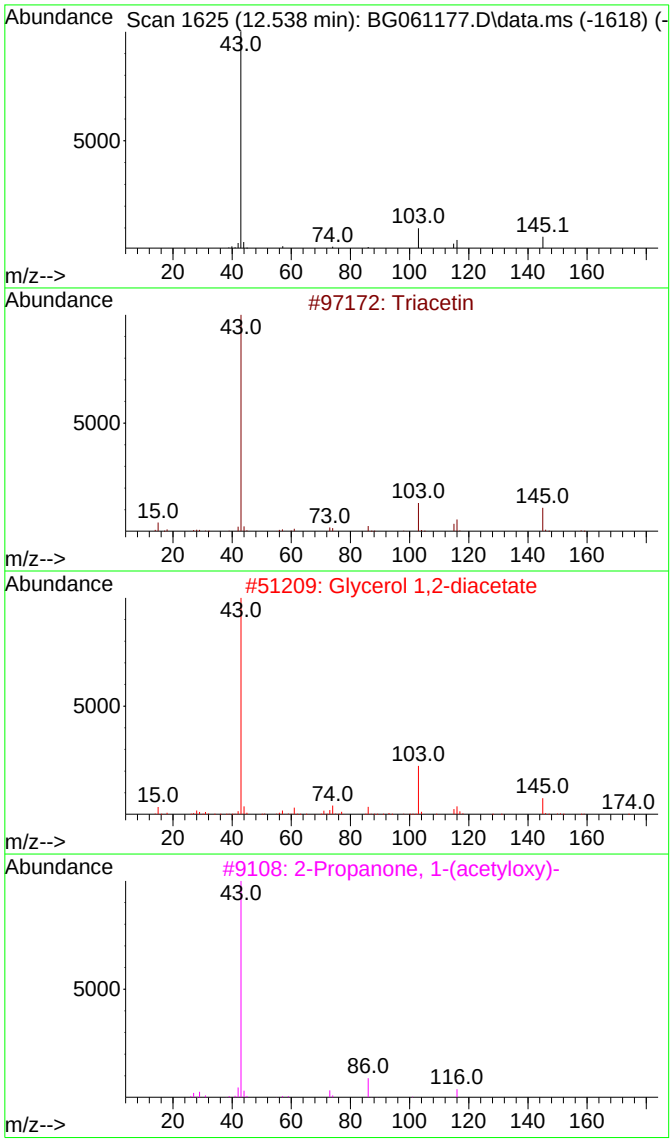
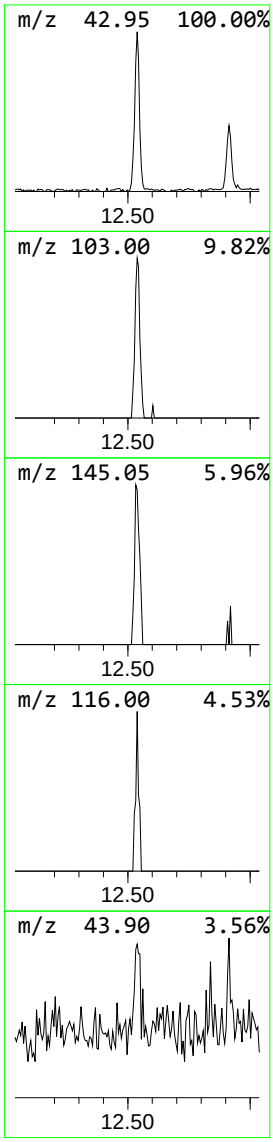
****

Peak Number 5 Triacetin Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.538	4.82 ng	40734	Naphthalene-d8	10.722

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacetin	218	C9H14O6	000102-76-1	78
2	Glycerol 1,2-diacetate	176	C7H12O5	000102-62-5	36
3	2-Propanone, 1-(acetyloxy)-	116	C5H8O3	000592-20-1	9
4	D-Xylononitrile, 2,3,4,5-tetraac...	315	C13H17NO8	013501-95-6	9
5	1,4-Dioxane-2,3-diol, diacetate	204	C8H12O6	015874-26-7	9





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
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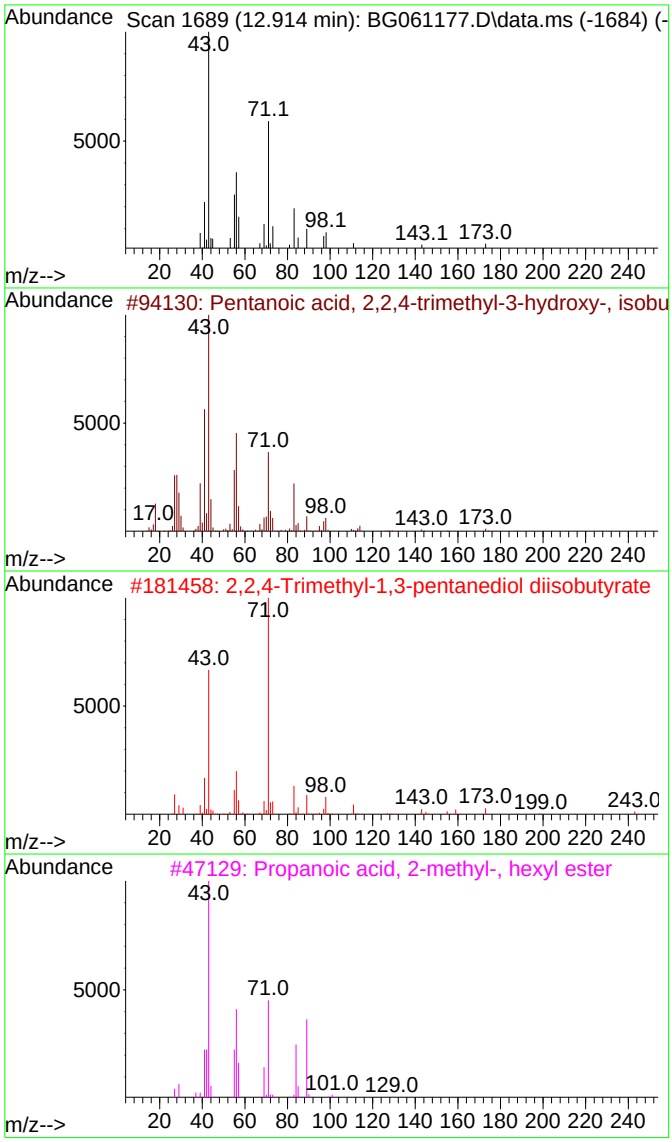
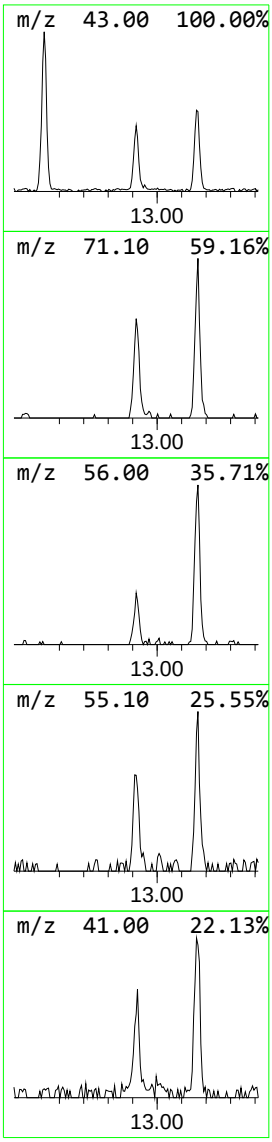
****

Peak Number 6 Pentanoic acid, 2,2,4-trime... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.914	3.77 ng	50077	Acenaphthene-d10	14.559

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanoic acid, 2,2,4-trimethyl-...	216	C12H24O3	244074-78-0	59
2	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	50
3	Propanoic acid, 2-methyl-, hexyl...	172	C10H20O2	002349-07-7	43
4	Butanoic acid, 1-methylhexyl ester	186	C11H22O2	039026-94-3	43
5	Decanoic acid, octyl ester	284	C18H36O2	002306-92-5	38





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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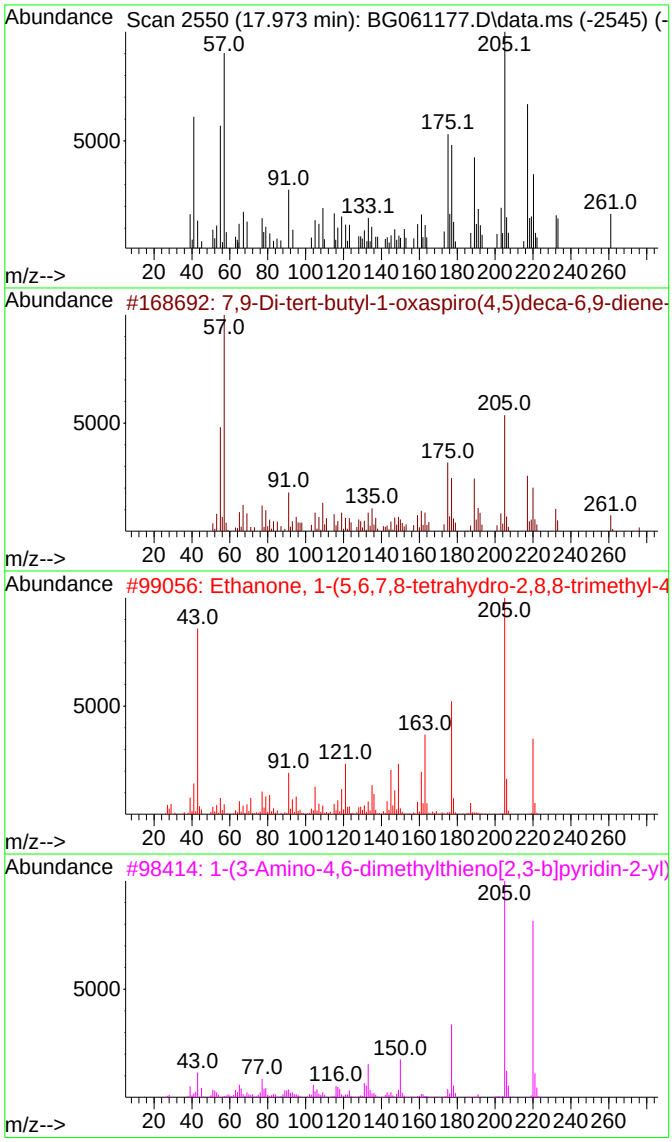
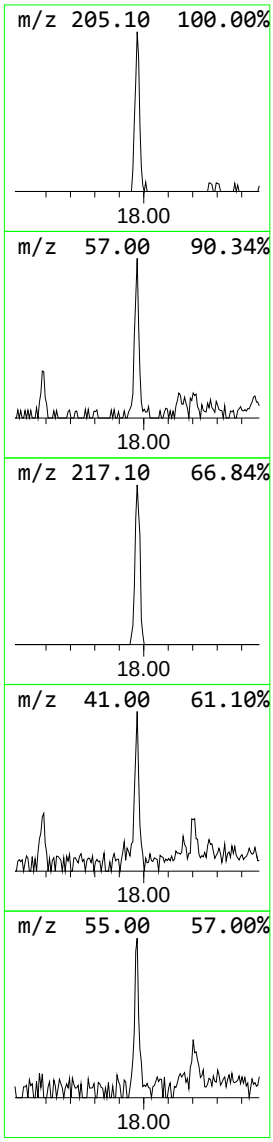
****

Peak Number 7 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.973	3.70 ng	72167	Phenanthrene-d10	17.303

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	87
2	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	50
3	1-(3-Amino-4,6-dimethylthieno[2,...	220	C11H12N2OS	052505-42-7	50
4	1,3-Pentadiene, 1,1-diphenyl-, (Z)-	220	C17H16	015295-31-5	42
5	2,5-Cyclohexadien-1-one, 2,6-bis...	232	C16H24O	006738-27-8	42





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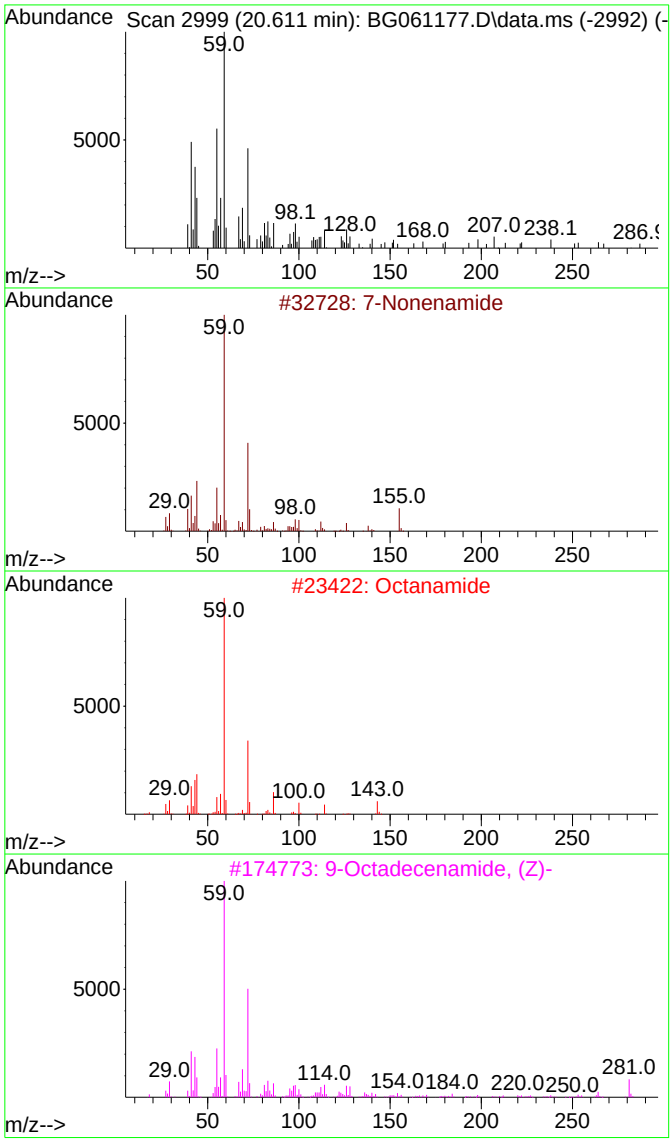
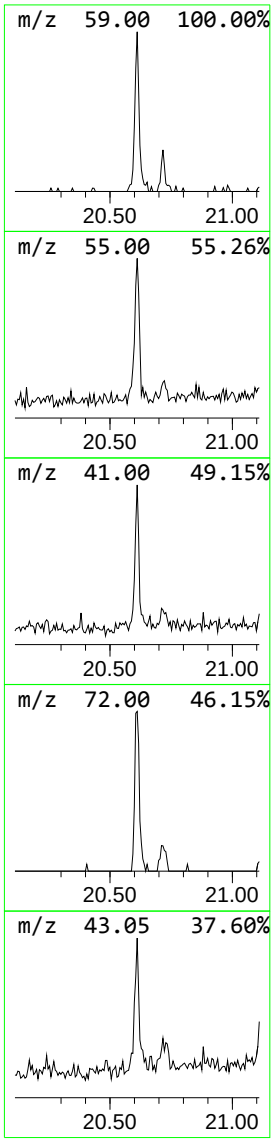
****

Peak Number 8 7-Nonenamide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.611	2.58 ng	66225	Chrysene-d12	21.563

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Nonenamide	155	C9H17NO	090949-53-4	72
2	Octanamide	143	C8H17NO	000629-01-6	72
3	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	72
4	Dodecanamide	199	C12H25NO	001120-16-7	64
5	Tetradecanamide	227	C14H29NO	000638-58-4	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051324\
Data File : BG061177.D
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Sample : P2449-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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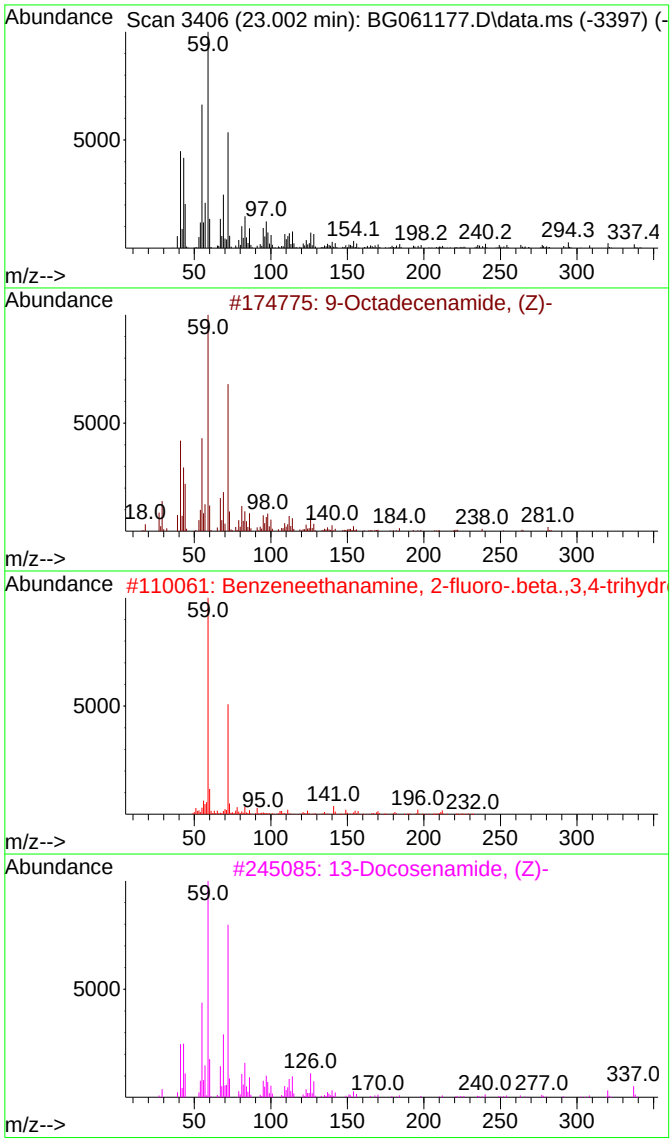
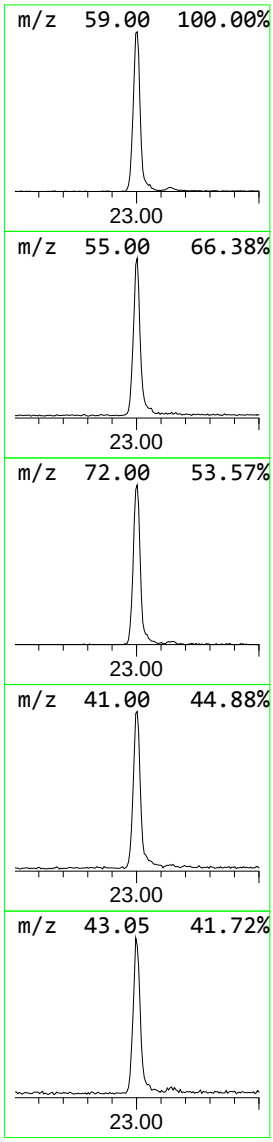
****

Peak Number 9 9-Octadecenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.002	44.36 ng	1138970	Chrysene-d12	21.563

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	62
2	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	59
3	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	53
4	Behenic amide	339	C22H45NO	003061-75-4	41
5	Palmitoleamide	253	C16H31NO	106010-22-4	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051324\
Data File : BG061177.D
Acq On : 13 May 2024 16:05
Operator : MA/JU
Sample : P2449-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1011UMR-RB240508-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.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
1-Pentene, 2-me...	3.073	7.3	ng	53285	1	7.926	146821	20.0
Butane, 2-metho...	3.149	195.7	ng	1436840	1	7.926	146821	20.0
1-Pentanol, 2-e...	7.990	5.6	ng	40879	1	7.926	146821	20.0
Phenol, 2-methoxy-	9.018	5.1	ng	37269	1	7.926	146821	20.0
Triacetin	12.538	4.8	ng	40734	2	10.722	168968	20.0
Pentanoic acid,...	12.914	3.8	ng	50077	3	14.559	265902	20.0
7,9-Di-tert-but...	17.973	3.7	ng	72167	4	17.303	389753	20.0
7-Nonenamide	20.611	2.6	ng	66225	5	21.563	513475	20.0
9-Octadecenamid...	23.002	44.4	ng	1138970	5	21.563	513475	20.0