LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051324\
Data File : BG061178.D
Acq On : 13 May 2024 16:46
Operator : MA/JU
Sample : P2450-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1011UMR-RB240507-01

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: BG061178.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.066	8	13	21	rVV6	14748	28709	1.08%	0.271%
2	3.143	21	26	43	rVB	841012	1146477	43.11%	10.821%
3	3.854	142	147	157	rVB	47947	68675	2.58%	0.648%
4	4.453	243	249	259	rVB	293605	416064	15.65%	3.927%
5	5.046	343	350	358	rVB	194489	275847	10.37%	2.604%
6	5.522	425	431	441	rVB	191640	293960	11.05%	2.775%
7	7.103	691	700	712	rVB	114172	199106	7.49%	1.879%
8	7.925	834	840	846	rBV	85910	139611	5.25%	1.318%
9	7.990	846	851	859	rVB	24514	41297	1.55%	0.390%
10	9.018	1020	1026	1030	rBV	27486	43671	1.64%	0.412%
11	9.083	1030	1037	1048	rVB	309305	538302	20.24%	5.081%
12	9.247	1060	1065	1070	rBV3	15914	27105	1.02%	0.256%
13	10.722	1307	1316	1323	rVB	96649	169705	6.38%	1.602%
14	11.098	1374	1380	1383	rBV3	19046	31936	1.20%	0.301%
15	11.133	1383	1386	1391	rVB	20594	29142	1.10%	0.275%
16	11.362	1419	1425	1434	rVB	18571	34613	1.30%	0.327%
17	12.538	1619	1625	1633	rBV	26684	39547	1.49%	0.373%
18	13.178	1726	1734	1741	rBV	716479	1134473	42.66%	10.708%
19	14.559	1963	1969	1978	rBV	147720	240031	9.03%	2.266%
20	15.375	2100	2108	2113	rVB2	31382	48995	1.84%	0.462%
21	16.051	2216	2223	2236	rBV	770045	1208020	45.43%	11.402%
22	17.303	2429	2436	2445	rBV	250535	380237	14.30%	3.589%
23	18.713	2672	2676	2682	rVB2	30227	38609	1.45%	0.364%
24	19.929	2876	2883	2890	rBV	1918386	2659281	100.00%	25.099%
25	21.257	3106	3109	3117	rVB2	50713	73020	2.75%	0.689%
26	21.562	3155	3161	3168	rVB	317525	493093	18.54%	4.654%
27	23.002	3398	3406	3418	rBV	211379	494255	18.59%	4.665%
28	24.682	3684	3692	3703	rBV3	107667	301206	11.33%	2.843%

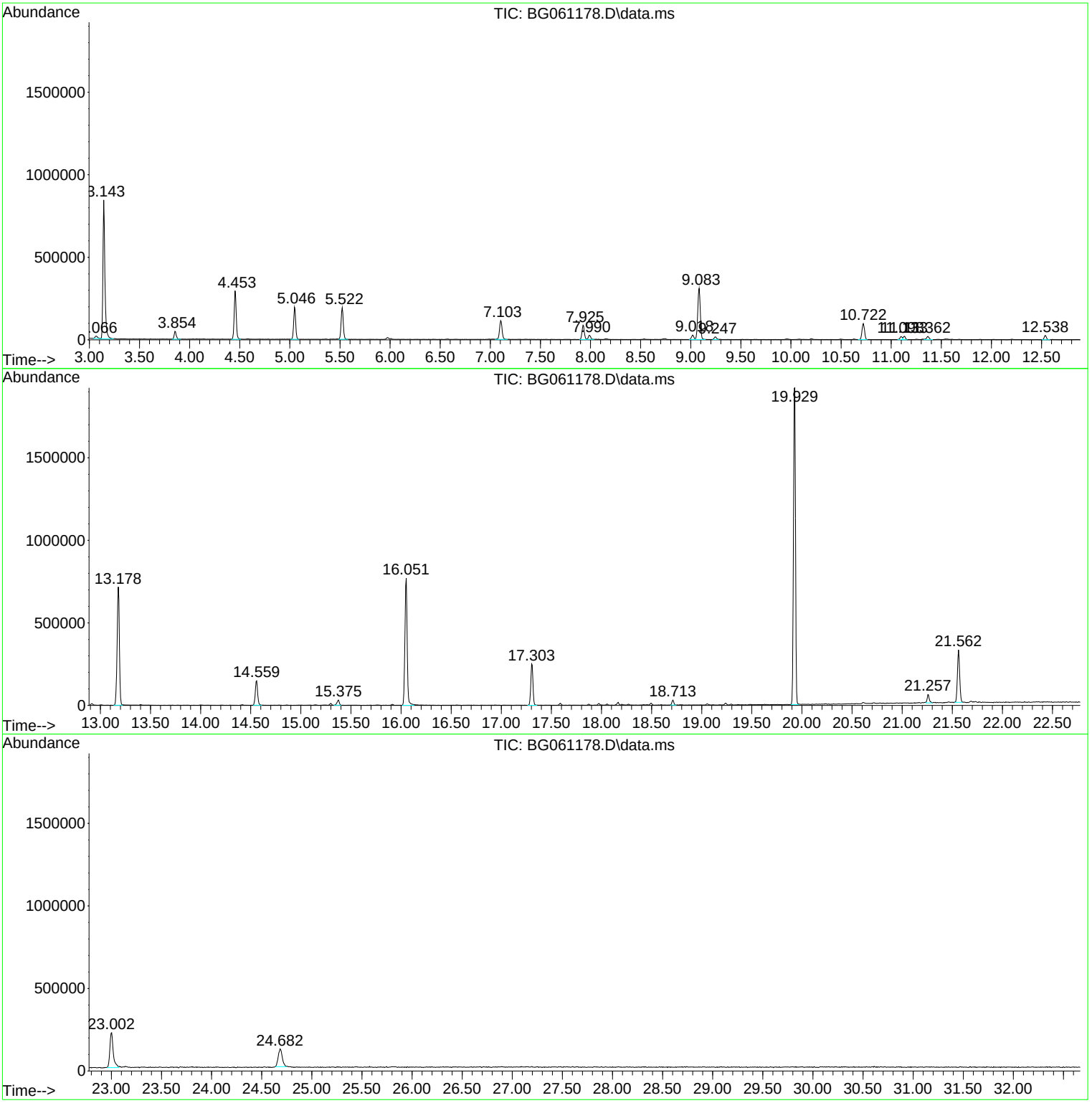
Sum of corrected areas: 10594987

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051324\
Data File : BG061178.D
Acq On : 13 May 2024 16:46
Operator : MA/JU
Sample : P2450-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1011UMR-RB240507-01

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051324\
Data File : BG061178.D
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Operator : MA/JU
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

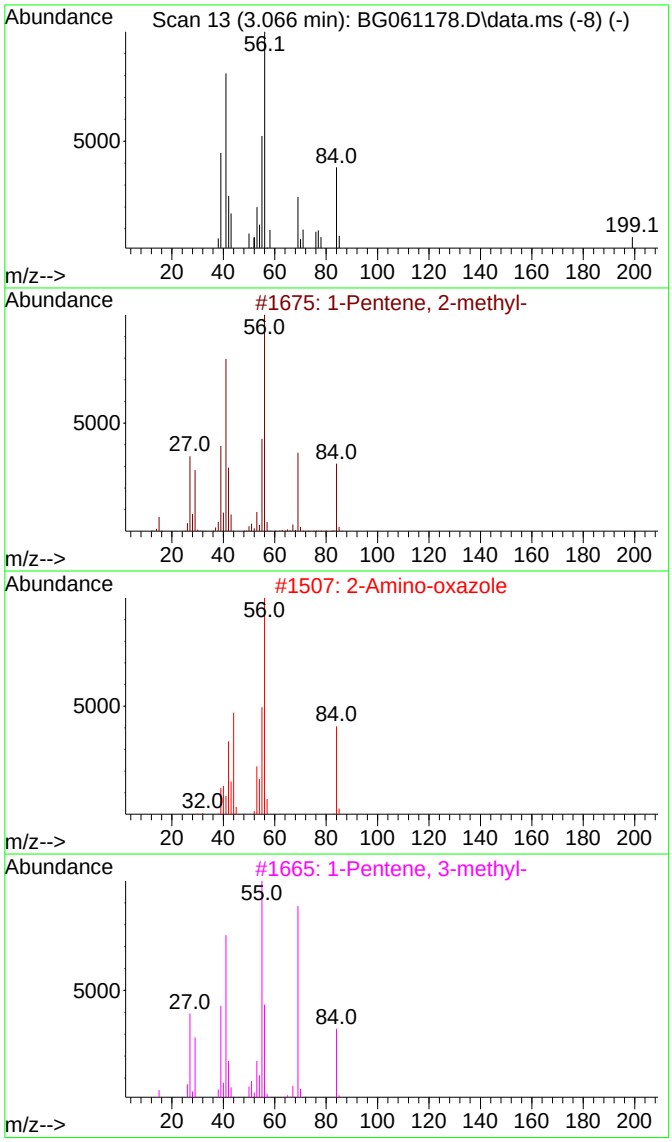
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

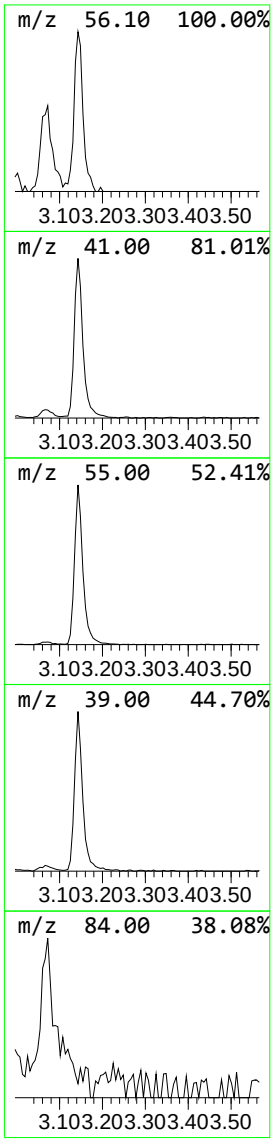
****

Peak Number 1 1-Pentene, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.066	4.11 ng	28709	1,4-Dichlorobenzene-d4	7.925

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	72
2	2-Amino-oxazole	84	C3H4N2O	004570-45-0	58
3	1-Pentene, 3-methyl-	84	C6H12	000760-20-3	53
4	Cyclohexane	84	C6H12	000110-82-7	47
5	Cyclopropane, 1-ethyl-2-methyl-,...	84	C6H12	019781-68-1	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051324\
Data File : BG061178.D
Acq On : 13 May 2024 16:46
Operator : MA/JU
Sample : P2450-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1011UMR-RB240507-01

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

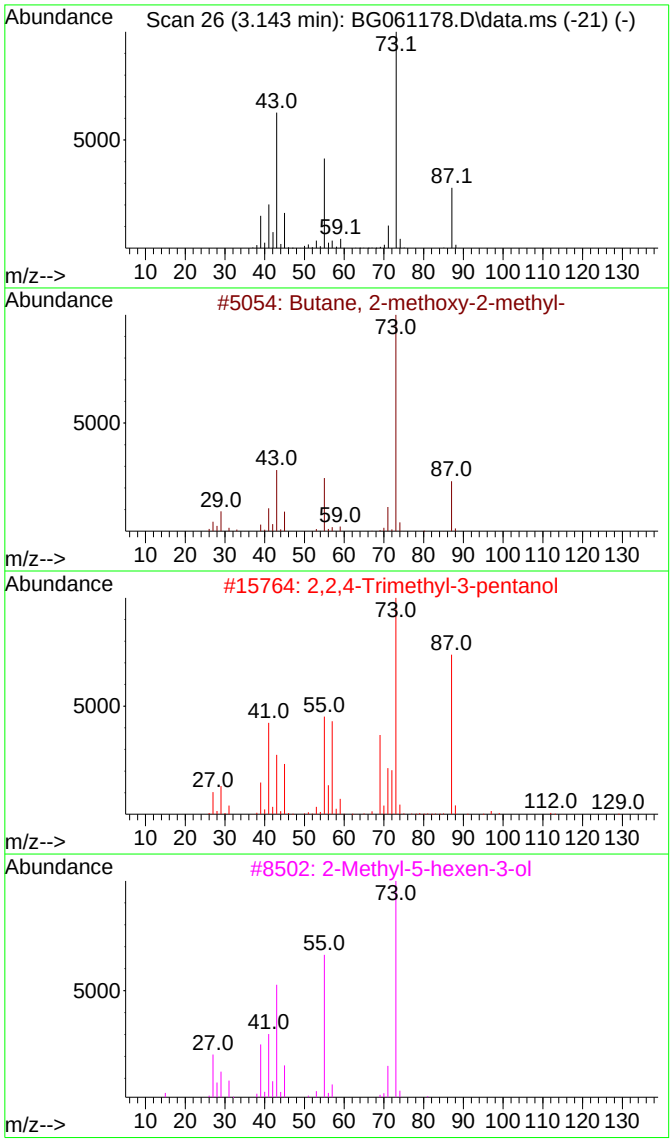
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

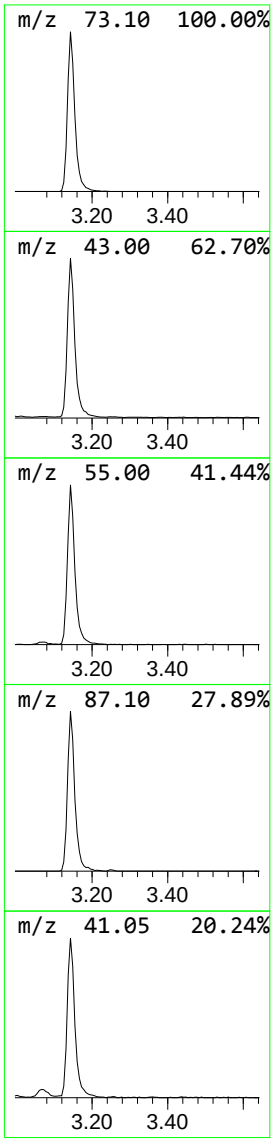
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.143	164.24 ng	1146480	1,4-Dichlorobenzene-d4	7.925

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	90
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	37
4	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	33
5	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	17





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Data File : BG061178.D
Acq On : 13 May 2024 16:46
Operator : MA/JU
Sample : P2450-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1011UMR-RB240507-01

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

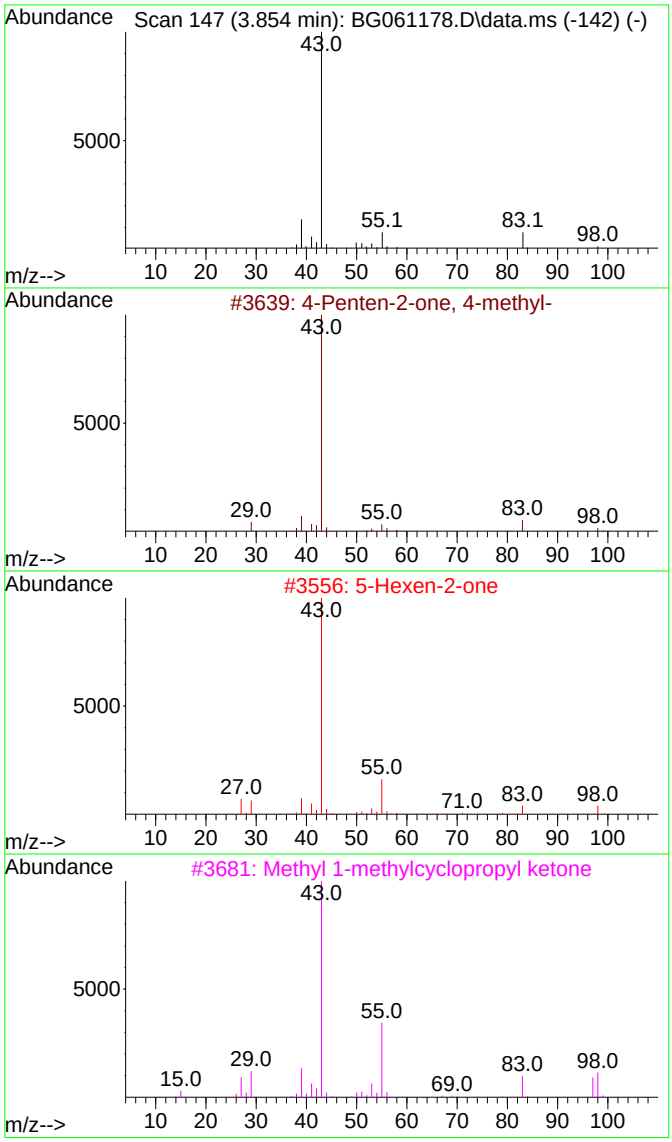
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

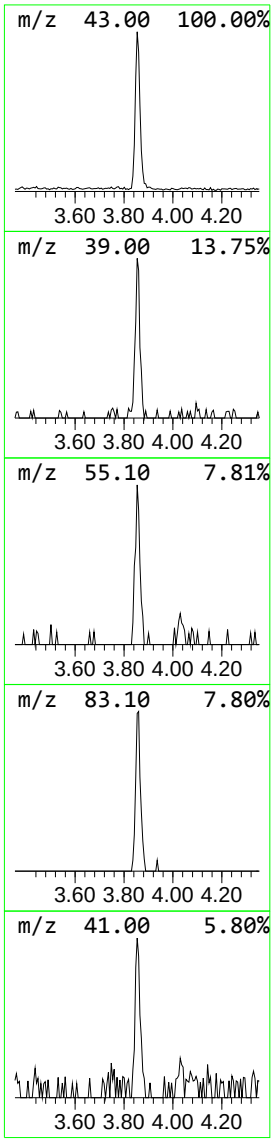
****

Peak Number 3 4-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.854	9.84 ng	68675	1,4-Dichlorobenzene-d4	7.925

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	53
2	5-Hexen-2-one	98	C6H10O	000109-49-9	49
3	Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	12
4	Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9
5	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	9





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Data File : BG061178.D
Acq On : 13 May 2024 16:46
Operator : MA/JU
Sample : P2450-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1011UMR-RB240507-01

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

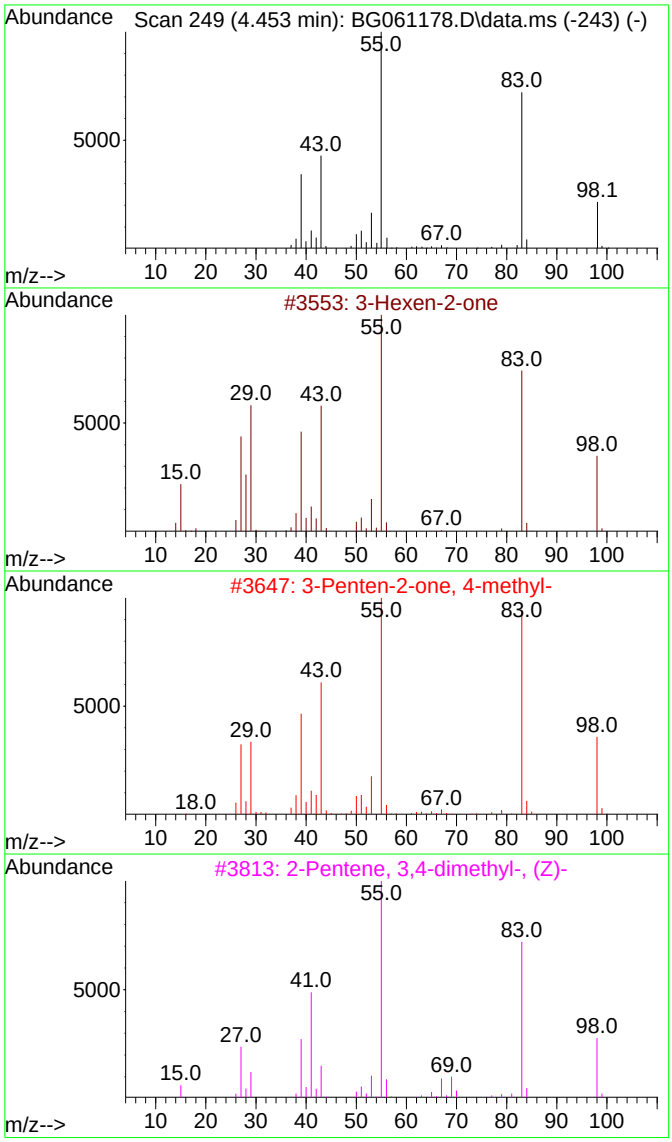
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

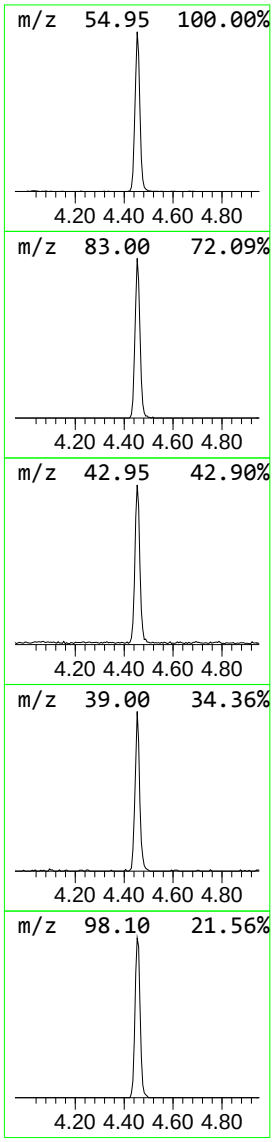
****

Peak Number 4 3-Hexen-2-one Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.453	59.60 ng	416064	1,4-Dichlorobenzene-d4	7.925

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-2-one	98	C6H10O	000763-93-9	90
2	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	78
3	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	72
4	2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	72
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051324\
Data File : BG061178.D
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Operator : MA/JU
Sample : P2450-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1011UMR-RB240507-01

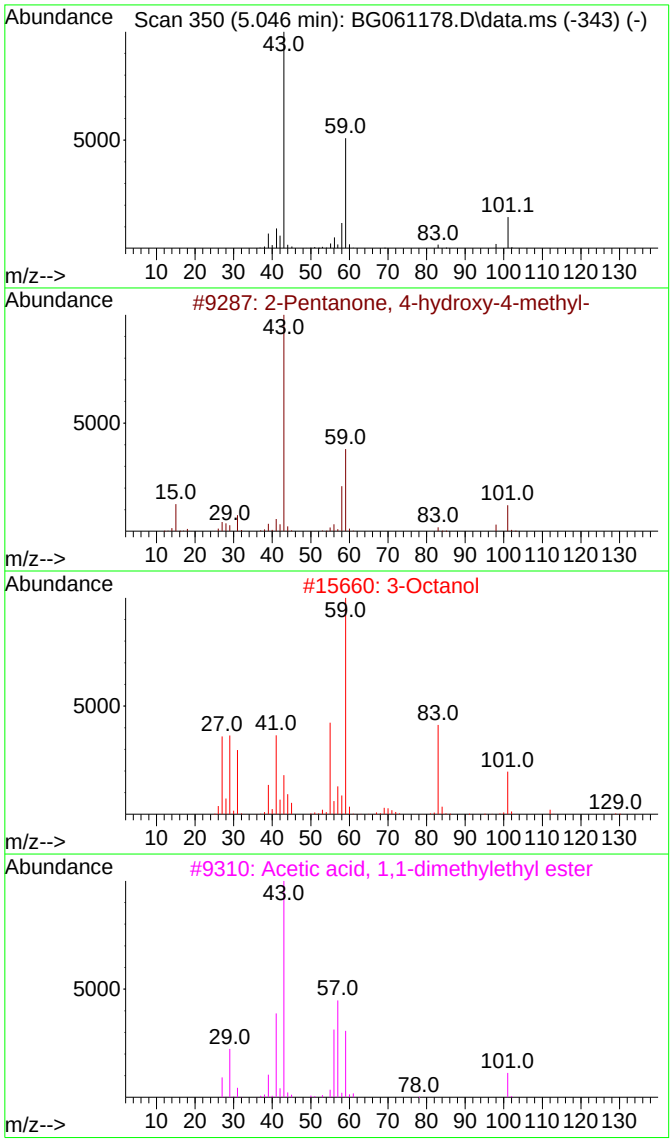
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

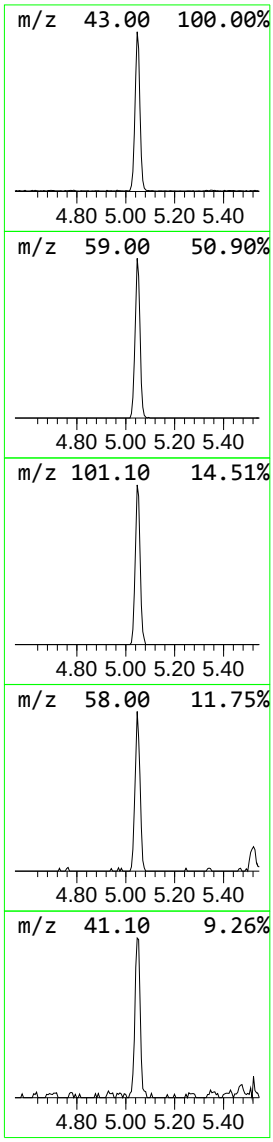
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.046	39.52 ng	275847	1,4-Dichlorobenzene-d4	7.925

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Octanol	130	C8H18O	000589-98-0	33
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





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Instrument :
BNA_G
ClientSampleId :
1011UMR-RB240507-01

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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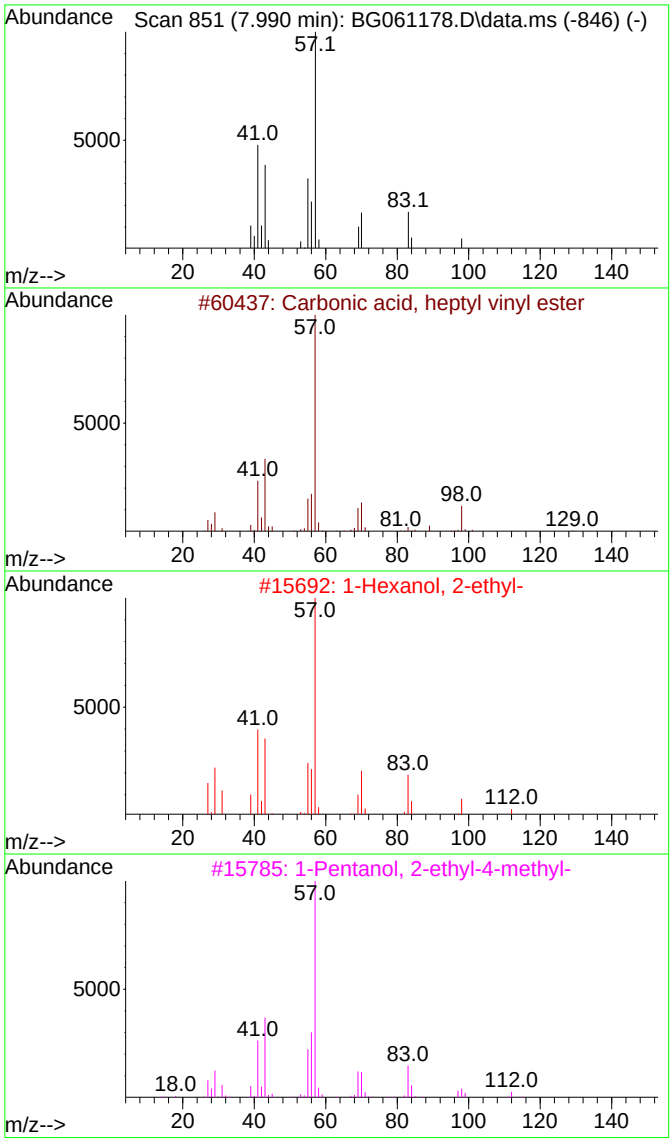
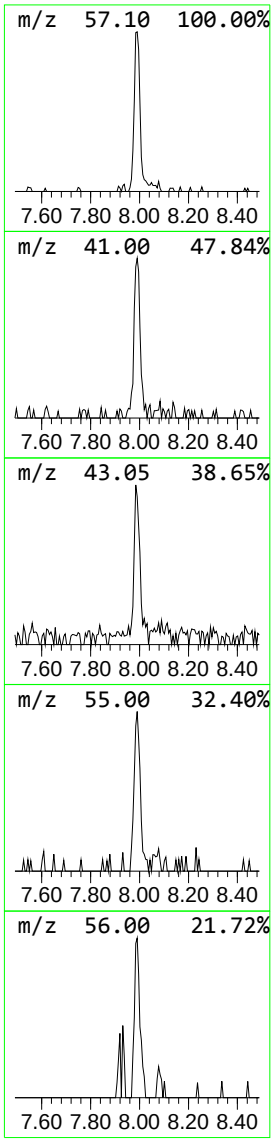
****
Peak Number 6 Carbonic acid, heptyl vinyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.990	5.92 ng	41297	1,4-Dichlorobenzene-d4	7.925

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	72
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
3	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	64
4	Carbonic acid, heptyl prop-1-en-...	200	C11H20O3	1000382-54-1	50
5	Oxalic acid, heptyl propyl ester	230	C12H22O4	1000309-26-0	42





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Data File : BG061178.D
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Sample : P2450-01
Misc :
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Instrument :
BNA_G
ClientSampleId :
1011UMR-RB240507-01

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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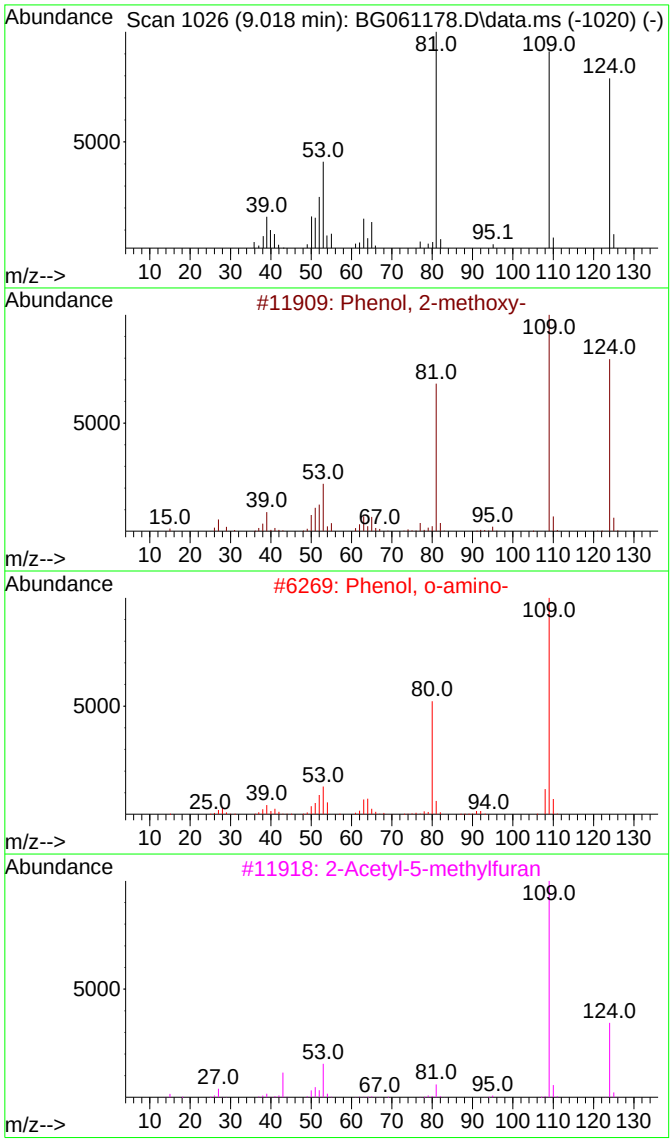
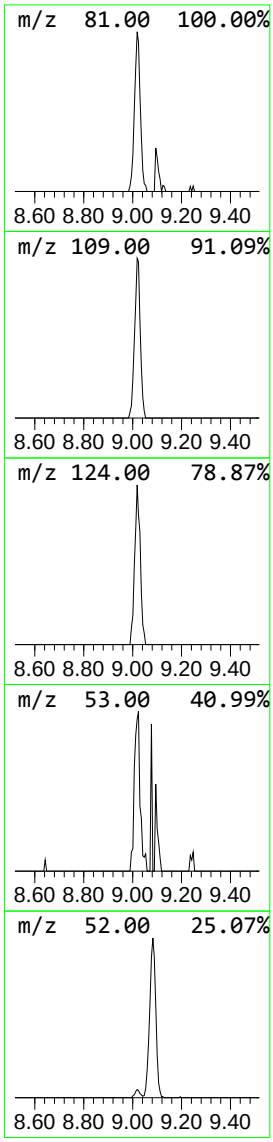
****

Peak Number 7 Phenol, 2-methoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.018	6.26 ng	43671	1,4-Dichlorobenzene-d4	7.925

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	94
2	Phenol, o-amino-	109	C6H7NO	000095-55-6	52
3	2-Acetyl-5-methylfuran	124	C7H8O2	001193-79-9	52
4	Mequinol	124	C7H8O2	000150-76-5	52
5	5-Ethyl-2-furaldehyde	124	C7H8O2	023074-10-4	50





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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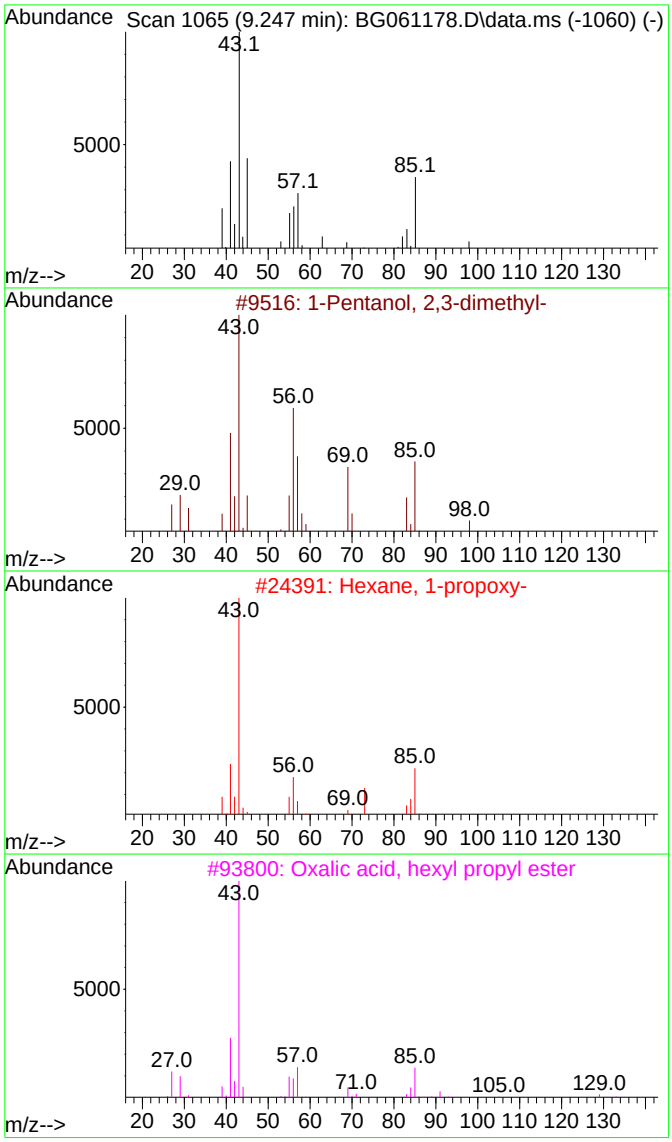
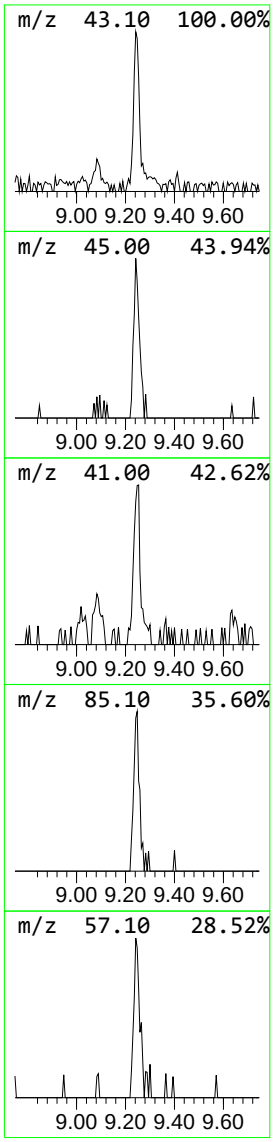
****

Peak Number 8 unknown9.247 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.247	3.88 ng	27105	1,4-Dichlorobenzene-d4	7.925

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentanol, 2,3-dimethyl-	116	C7H16O	010143-23-4	25
2	Hexane, 1-propoxy-	144	C9H20O	053685-78-2	17
3	Oxalic acid, hexyl propyl ester	216	C11H20O4	1000309-25-9	16
4	Oxalic acid, butyl isohexyl ester	230	C12H22O4	1000309-32-7	16
5	O-Hexylhydroxylamine	117	C6H15NO	1000426-05-8	10





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Operator : MA/JU
Sample : P2450-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

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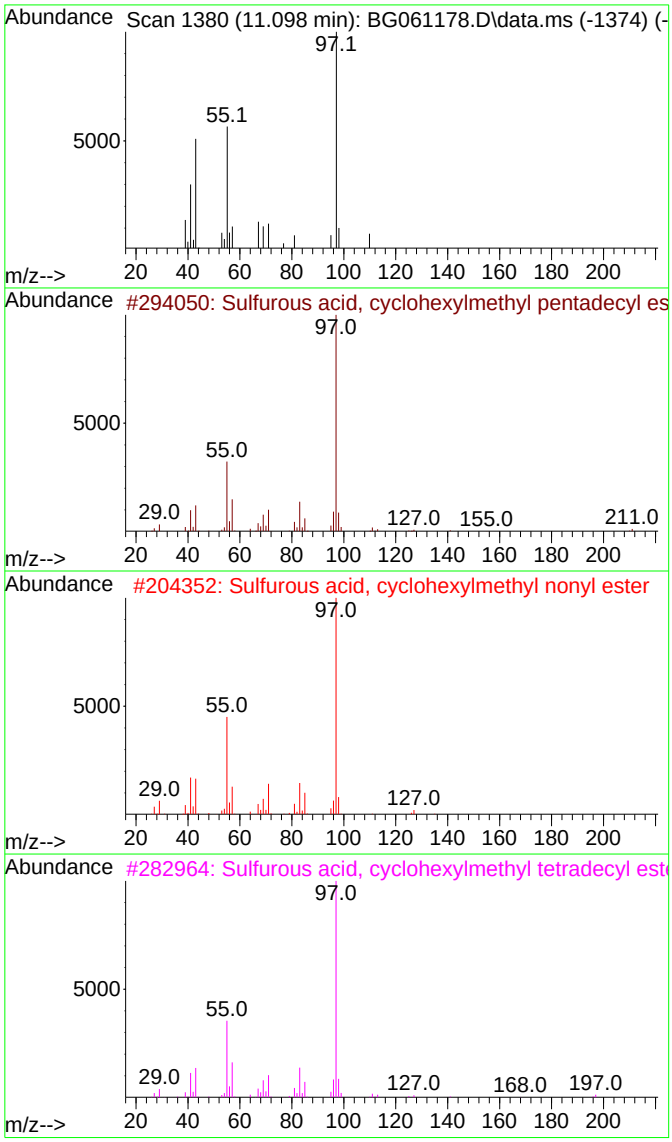
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

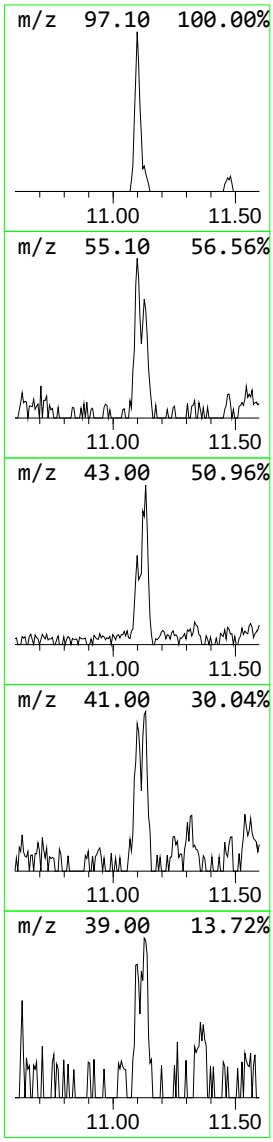
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Sulfurous acid, cyclohexylm... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.098	3.76 ng	31936	Naphthalene-d8	10.722

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, cyclohexylmethyl...	388	C22H44O3S	1000309-22-3	72
2	Sulfurous acid, cyclohexylmethyl...	304	C16H32O3S	1000309-21-8	72
3	Sulfurous acid, cyclohexylmethyl...	374	C21H42O3S	1000309-22-2	72
4	Sulfurous acid, cyclohexylmethyl...	262	C13H26O3S	1000309-21-5	72
5	Oxalic acid, cyclohexylmethyl et...	214	C11H18O4	1000309-68-0	64





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Data File : BG061178.D
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Operator : MA/JU
Sample : P2450-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1011UMR-RB240507-01

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

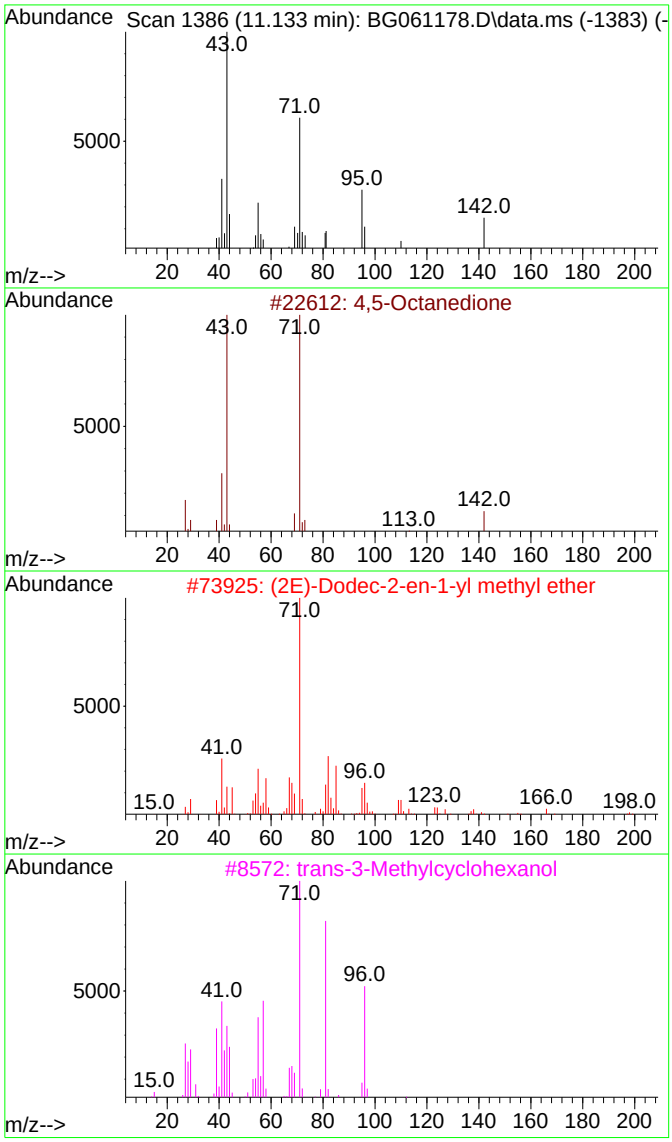
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

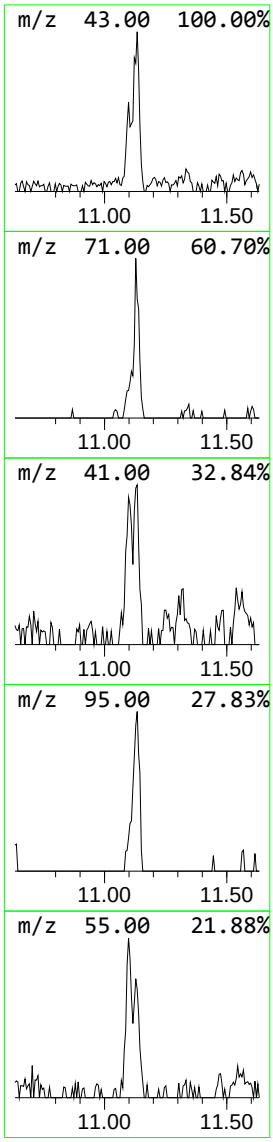
****

Peak Number 10 unknown11.133 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.133	3.43 ng	29142	Naphthalene-d8	10.722

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,5-Octanedione	142	C8H14O2	005455-24-3	47
2	(2E)-Dodec-2-en-1-yl methyl ether	198	C13H26O	1000334-06-3	40
3	trans-3-Methylcyclohexanol	114	C7H14O	007443-55-2	28
4	Ether, methyl 1-octadecenyl	282	C19H38O	026537-06-4	25
5	Ethanedioic acid, bis(3-methylbu...	230	C12H22O4	002051-00-5	12





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Acq On : 13 May 2024 16:46
Operator : MA/JU
Sample : P2450-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1011UMR-RB240507-01

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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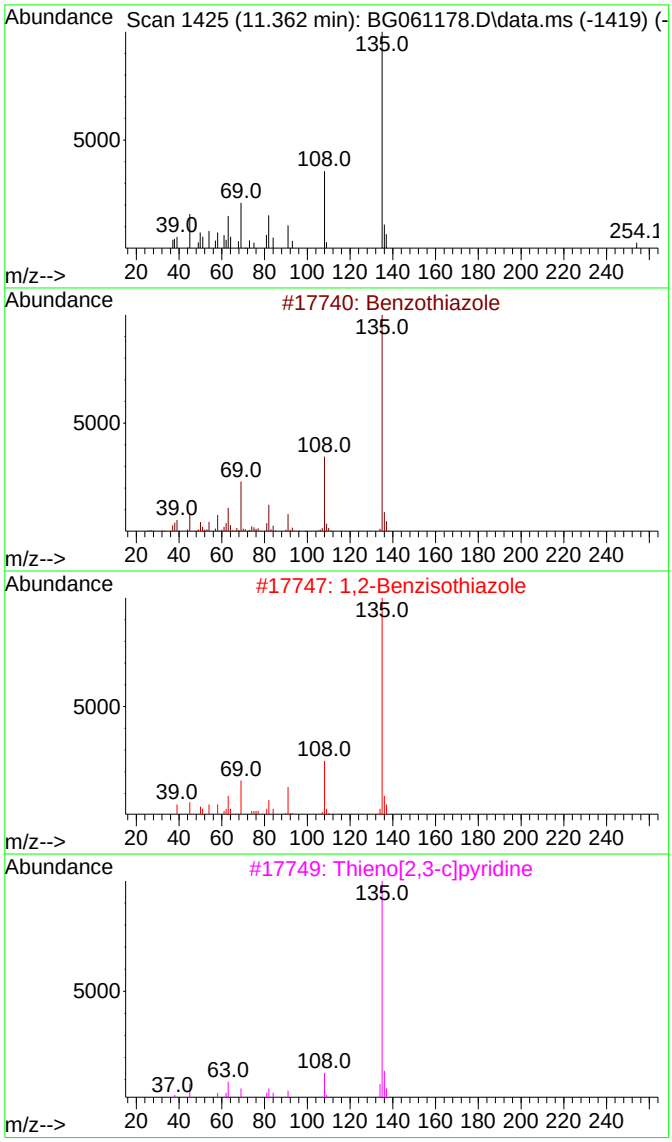
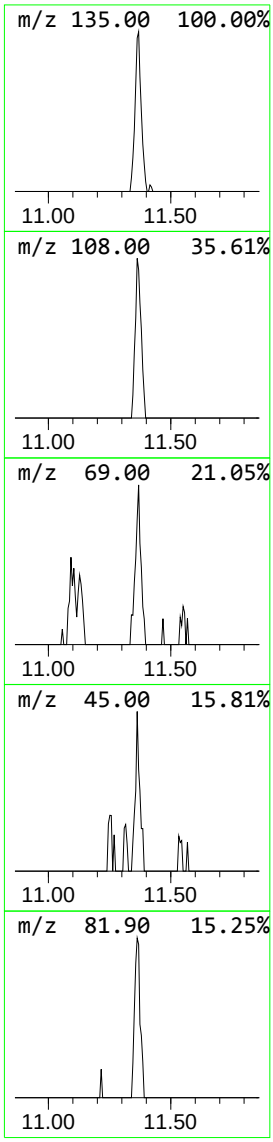
Peak Number 11 Benzothiazole Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.363	4.08 ng	34613	Naphthalene-d8	10.722

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzothiazole	135	C7H5NS	000095-16-9	90
2	1,2-Benzisothiazole	135	C7H5NS	000272-16-2	86
3	Thieno[2,3-c]pyridine	135	C7H5NS	000272-12-8	72
4	Thieno[3,2-c]pyridine	135	C7H5NS	000272-14-0	68
5	1H-Pyrazolo[3,4-d]pyrimidin-4-amine	135	C5H5N5	002380-63-4	64





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Acq On : 13 May 2024 16:46
Operator : MA/JU
Sample : P2450-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1011UMR-RB240507-01

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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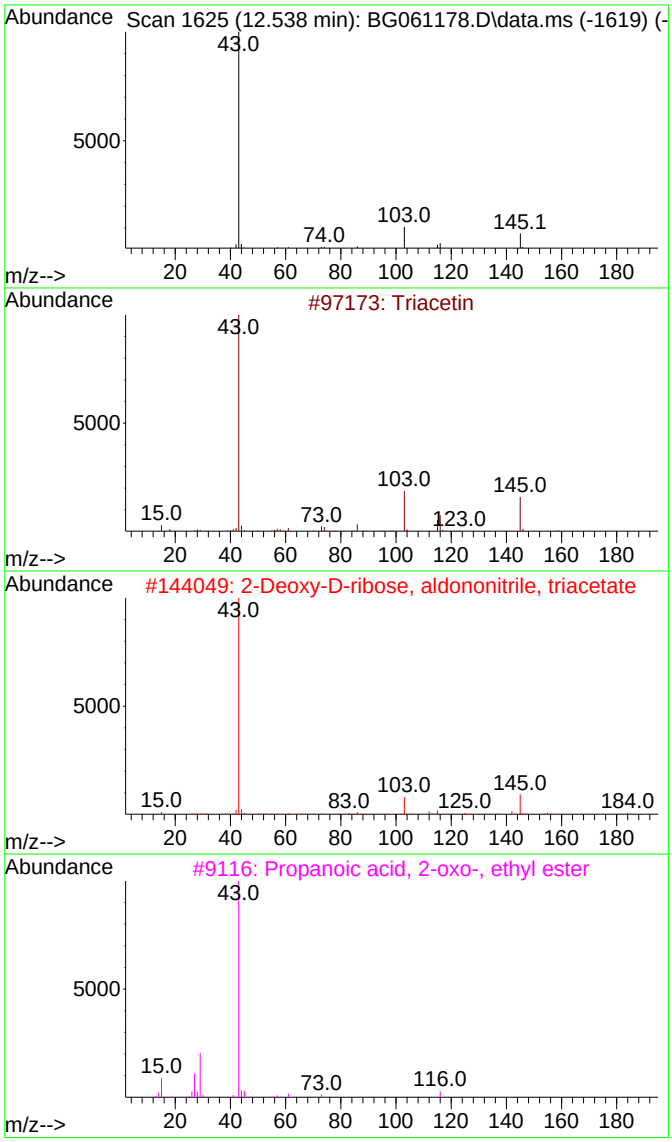
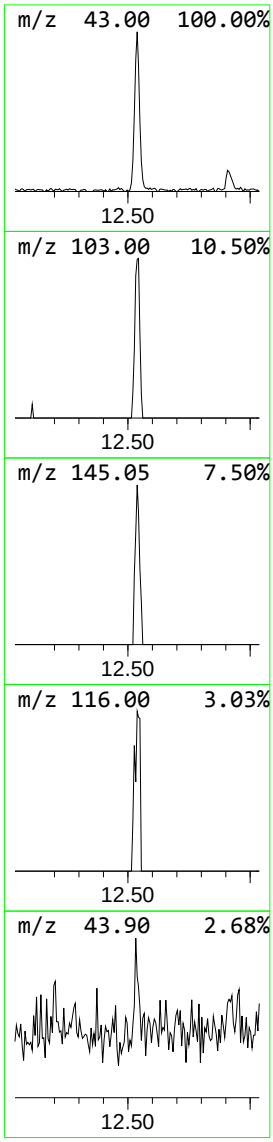
Peak Number 12 Triacetin Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.538	4.66 ng	39547	Naphthalene-d8	10.722

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacetin	218	C9H14O6	000102-76-1	74
2	2-Deoxy-D-ribose, aldononitrile,...	257	C11H15NO6	1000380-43-1	38
3	Propanoic acid, 2-oxo-, ethyl ester	116	C5H8O3	000617-35-6	32
4	1,2,3,4-Butanetetrol, tetraaceta...	290	C12H18O8	007208-40-4	9
5	Glycerol 1,2-diacetate	176	C7H12O5	000102-62-5	9





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Data File : BG061178.D
Acq On : 13 May 2024 16:46
Operator : MA/JU
Sample : P2450-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1011UMR-RB240507-01

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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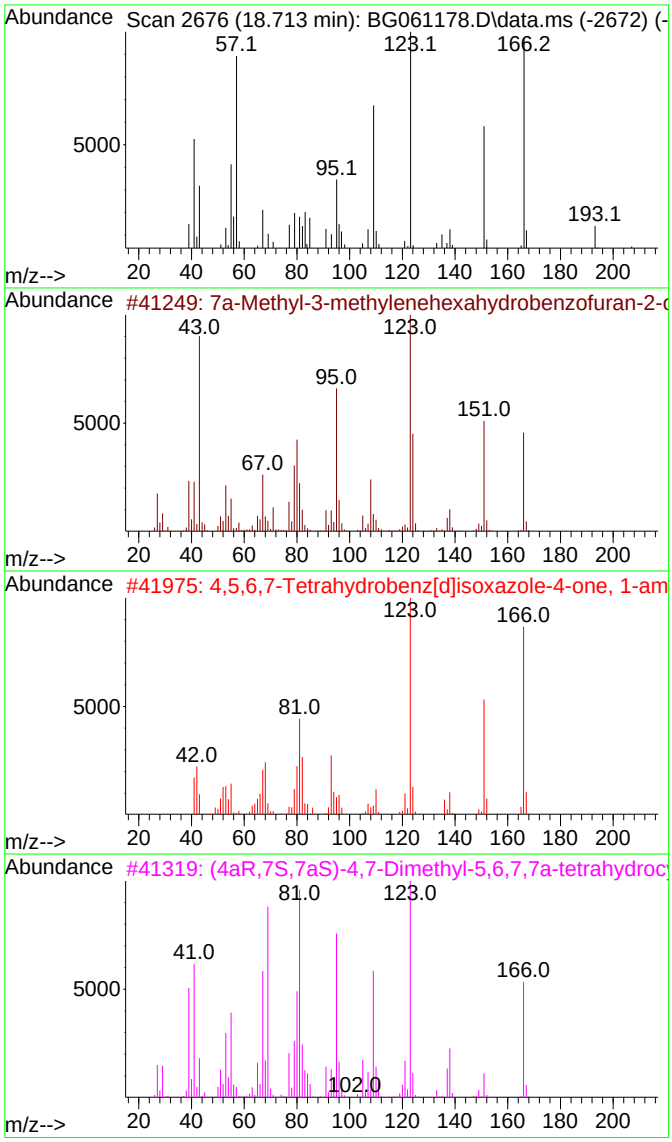
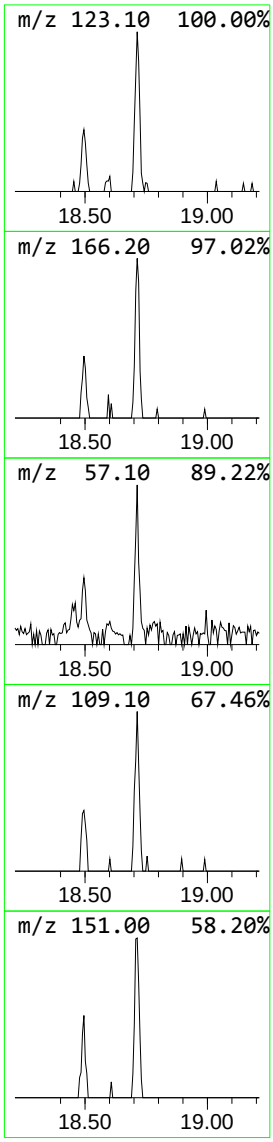
Peak Number 13 7a-Methyl-3-methylenehexahy... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.713	2.03 ng	38609	Phenanthrene-d10	17.303

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7a-Methyl-3-methylenehexahydrobe...	166	C10H14O2	067498-53-7	68
2	4,5,6,7-Tetrahydrobenz[d]isoxazo...	166	C8H10N2O2	1000131-45-3	62
3	(4aR,7S,7aS)-4,7-Dimethyl-5,6,7,...	166	C10H14O2	021651-53-6	59
4	l-Alanine, N-(3-fluorobenzoyl)-,...	239	C12H14FNO3	1000314-11-1	50
5	Phenol, 3-methoxy-2,5,6-trimethyl-	166	C10H14O2	034883-03-9	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051324\
Data File : BG061178.D
Acq On : 13 May 2024 16:46
Operator : MA/JU
Sample : P2450-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1011UMR-RB240507-01

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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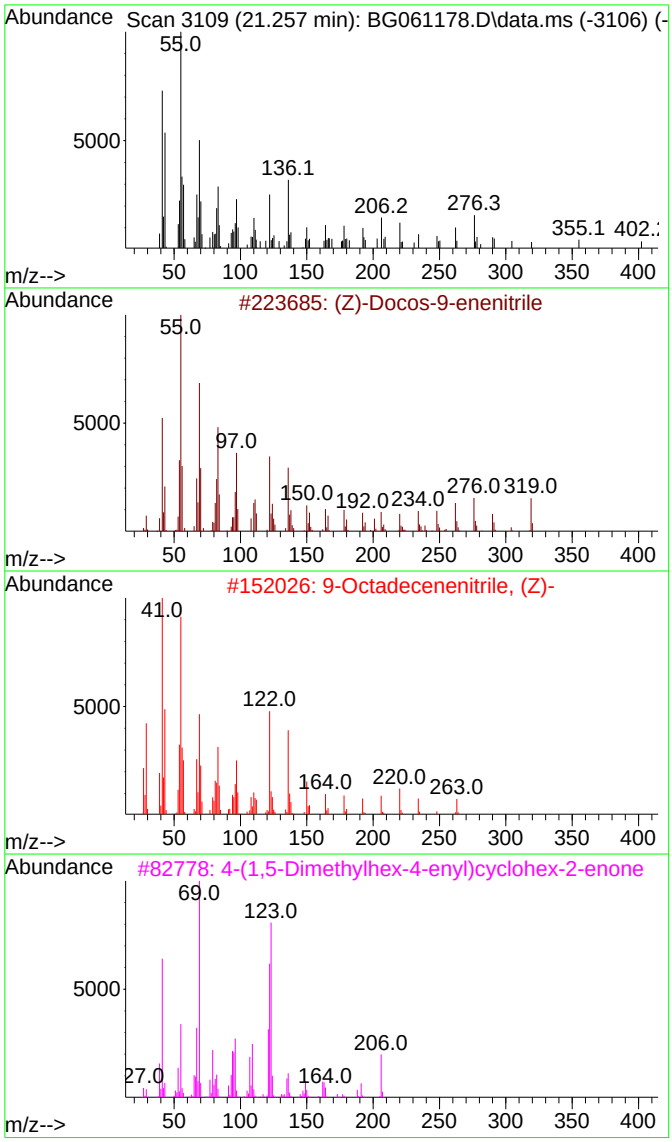
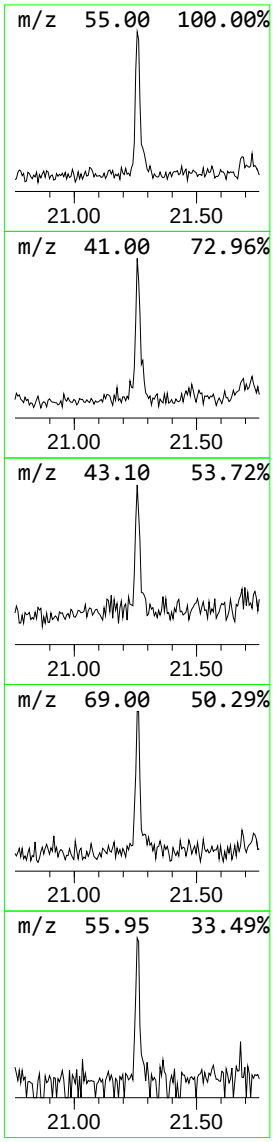
Peak Number 14 (Z)-Docos-9-enenitrile Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.257	2.96 ng	73020	Chrysene-d12	21.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(Z)-Docos-9-enenitrile	319	C22H41N	1000465-48-0	76
2	9-Octadecenenitrile, (Z)-	263	C18H33N	000112-91-4	46
3	4-(1,5-Dimethylhex-4-enyl)cycloh...	206	C14H22O	001723-80-4	35
4	Palmitoleonitrile	235	C16H29N	056617-97-1	27
5	Propanenitrile, 3-[1,1-diethyl-4...	262	C16H26N2O	1000277-29-8	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051324\
Data File : BG061178.D
Acq On : 13 May 2024 16:46
Operator : MA/JU
Sample : P2450-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1011UMR-RB240507-01

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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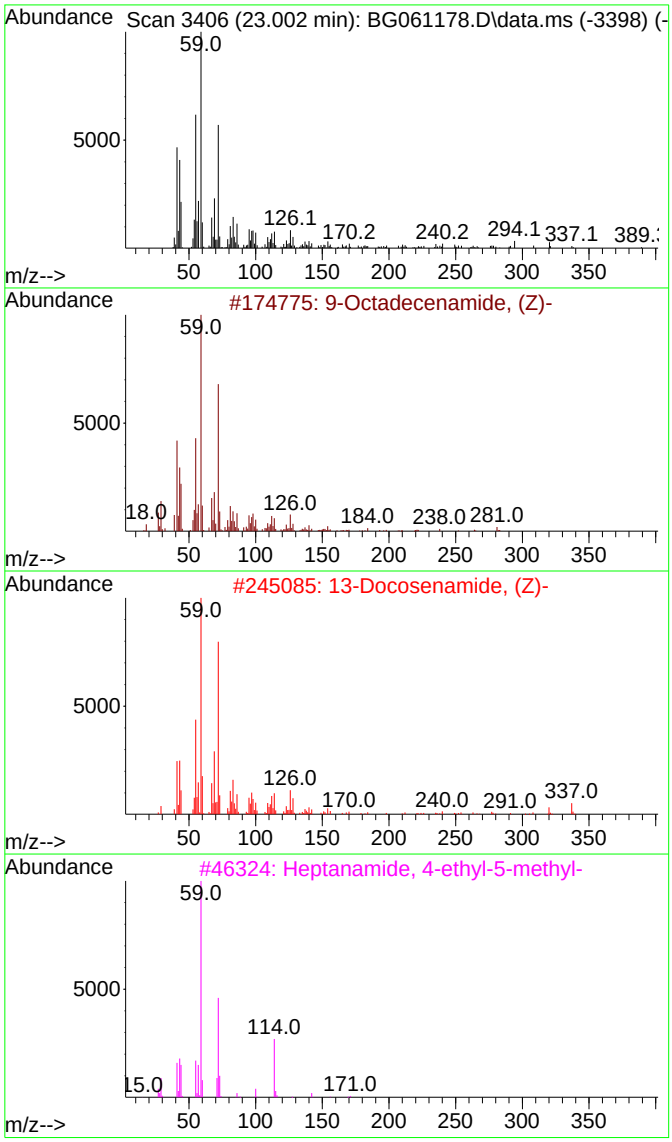
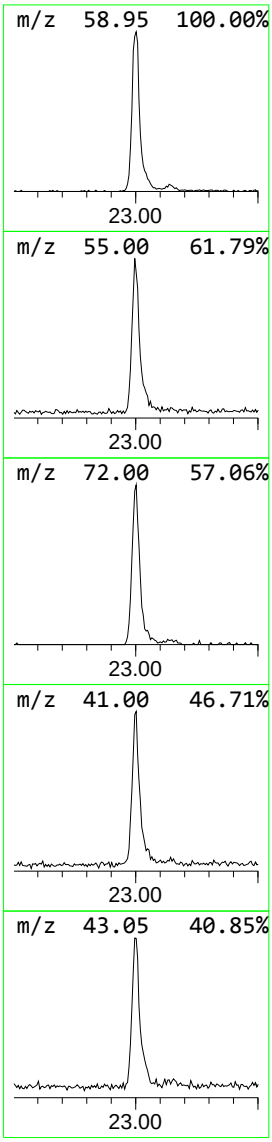
Peak Number 15 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.002	20.05 ng	494255	Chrysene-d12	21.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
2	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	81
3	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	80
4	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	64
5	2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051324\
Data File : BG061178.D
Acq On : 13 May 2024 16:46
Operator : MA/JU
Sample : P2450-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1011UMR-RB240507-01

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...	3.066	4.1	ng	28709	1	7.925	139611	20.0
Butane, 2-metho...	3.143	164.2	ng	1146480	1	7.925	139611	20.0
4-Penten-2-one,...	3.854	9.8	ng	68675	1	7.925	139611	20.0
3-Hexen-2-one	4.453	59.6	ng	416064	1	7.925	139611	20.0
2-Pentanone, 4-...	5.046	39.5	ng	275847	1	7.925	139611	20.0
Carbonic acid, ...	7.990	5.9	ng	41297	1	7.925	139611	20.0
Phenol, 2-methoxy-	9.018	6.3	ng	43671	1	7.925	139611	20.0
unknown9.247	9.247	3.9	ng	27105	1	7.925	139611	20.0
Sulfurous acid,...	11.098	3.8	ng	31936	2	10.722	169705	20.0
unknown11.133	11.133	3.4	ng	29142	2	10.722	169705	20.0
Benzothiazole	11.363	4.1	ng	34613	2	10.722	169705	20.0
Triacetin	12.538	4.7	ng	39547	2	10.722	169705	20.0
7a-Methyl-3-met...	18.713	2.0	ng	38609	4	17.303	380237	20.0
(Z)-Docos-9-ene...	21.257	3.0	ng	73020	5	21.562	493093	20.0
9-Octadecenamid...	23.002	20.1	ng	494255	5	21.562	493093	20.0