LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051524\
Data File : BG061203.D
Acq On : 15 May 2024 12:56
Operator : MA/JU
Sample : P2450-01
Misc :
ALS Vial : 6 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: BG061203.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	7	13	21	rBV6	12643	28298	1.21%	0.242%
2	3.142	21	26	40	rVB	650818	1013110	43.31%	8.663%
3	4.458	243	250	260	rVB	428599	639335	27.33%	5.467%
4	5.052	345	351	359	rVB	293370	430448	18.40%	3.681%
5	5.522	425	431	444	rVB	209516	332150	14.20%	2.840%
6	7.108	692	701	710	rVB	118534	218448	9.34%	1.868%
7	7.925	833	840	846	rBV	95860	156825	6.70%	1.341%
8	7.989	846	851	865	rVB3	18170	35488	1.52%	0.303%
9	9.018	1017	1026	1031	rBV2	28918	52406	2.24%	0.448%
10	9.088	1031	1038	1051	rVB	344416	618413	26.44%	5.288%
11	9.247	1060	1065	1070	rBV3	14184	24117	1.03%	0.206%
12	10.721	1308	1316	1328	rVB	124403	215000	9.19%	1.838%
13	11.368	1421	1426	1435	rVB2	17974	28888	1.23%	0.247%
14	12.537	1620	1625	1630	rBV	30487	45788	1.96%	0.392%
15	12.919	1685	1690	1700	rBV3	23272	51696	2.21%	0.442%
16	13.177	1725	1734	1743	rBV	931986	1488797	63.65%	12.730%
17	14.558	1962	1969	1977	rBV	196641	305871	13.08%	2.615%
18	15.375	2101	2108	2113	rVB3	33404	55162	2.36%	0.472%
19	16.050	2216	2223	2240	rBV	825996	1270809	54.33%	10.866%
20	17.308	2430	2437	2446	rBV	247153	384415	16.43%	3.287%
21	17.972	2545	2550	2554	rBV2	47618	57559	2.46%	0.492%
22	18.495	2634	2639	2644	rVB4	20047	26984	1.15%	0.231%
23	18.712	2671	2676	2681	rBV2	29740	36821	1.57%	0.315%
24	19.476	2803	2806	2814	rVB7	12700	24837	1.06%	0.212%
25	19.928	2877	2883	2889	rBV	1827640	2339185	100.00%	20.002%
26	20.028	2895	2900	2905	rBV3	14075	29007	1.24%	0.248%
27	20.727	3014	3019	3026	rBV3	27066	58025	2.48%	0.496%
28	21.262	3105	3110	3114	rVB3	24653	30965	1.32%	0.265%
29	21.421	3131	3137	3142	rBV3	22907	44793	1.91%	0.383%
30	21.568	3156	3162	3169	rVB	282485	456182	19.50%	3.901%
31	23.001	3398	3406	3422	rBV2	315501	719236	30.75%	6.150%
32	24.693	3683	3694	3704	rBV	148639	475858	20.34%	4.069%

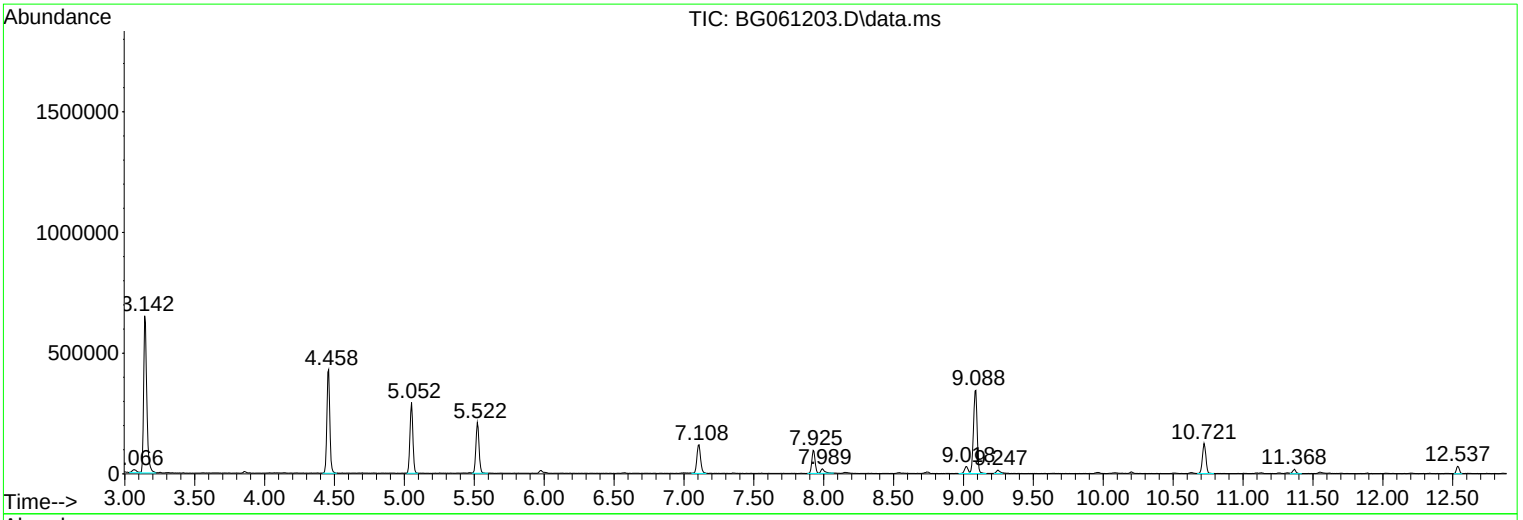
Sum of corrected areas: 11694916

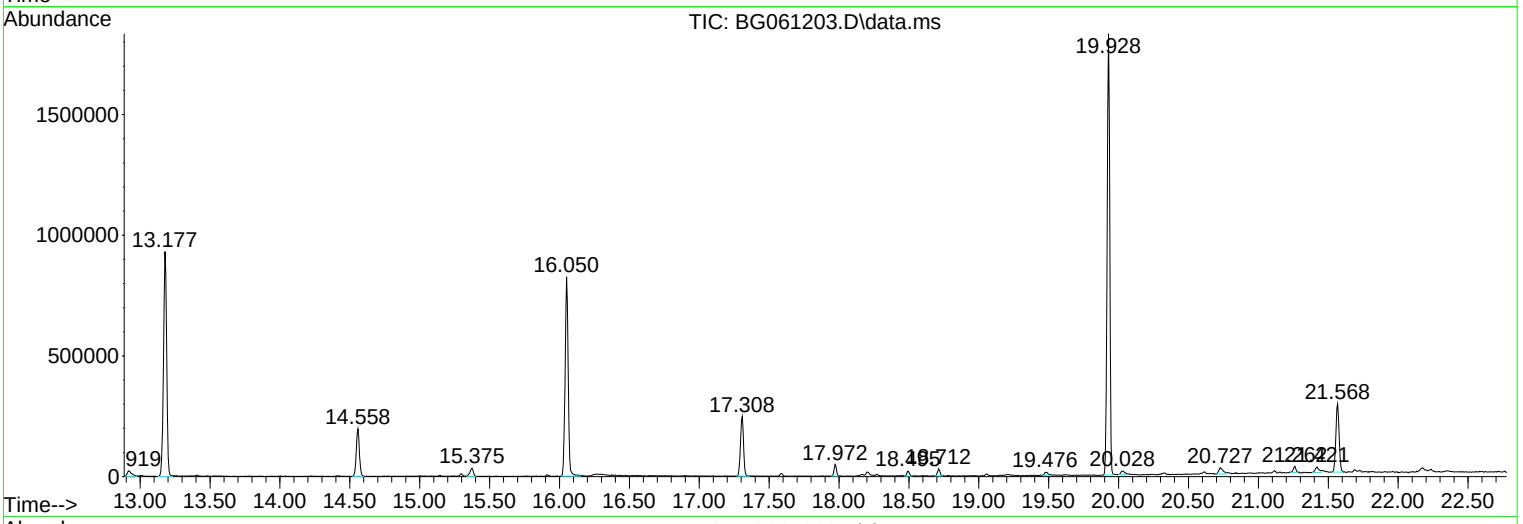
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051524\
Data File : BG061203.D
Acq On : 15 May 2024 12:56
Operator : MA/JU
Sample : P2450-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

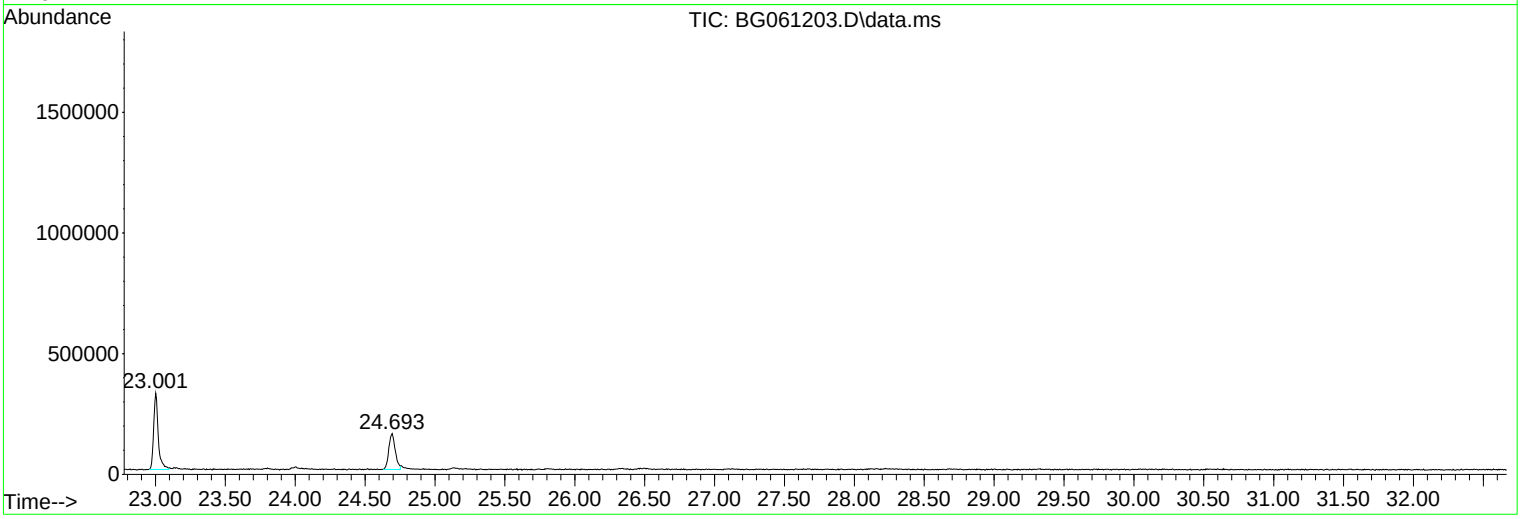
Instrument :
BNA_G
ClientSampleId :
1011UMR-RB240507-01

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\BG051524\
Data File : BG061203.D
Acq On : 15 May 2024 12:56
Operator : MA/JU
Sample : P2450-01
Misc :
ALS Vial : 6 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

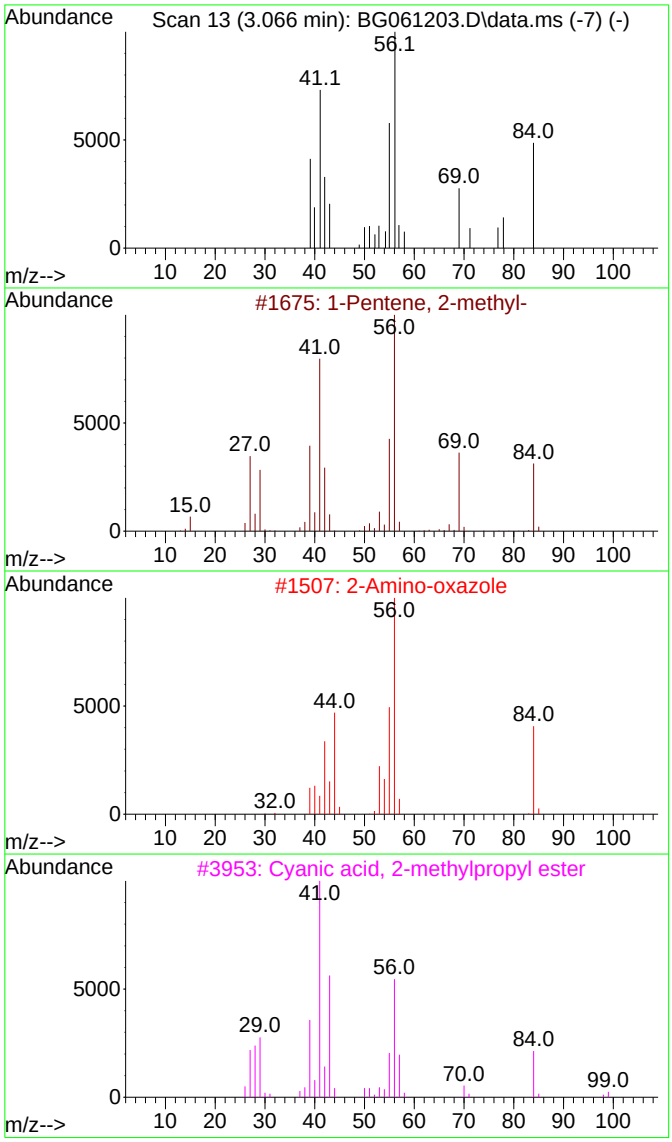
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

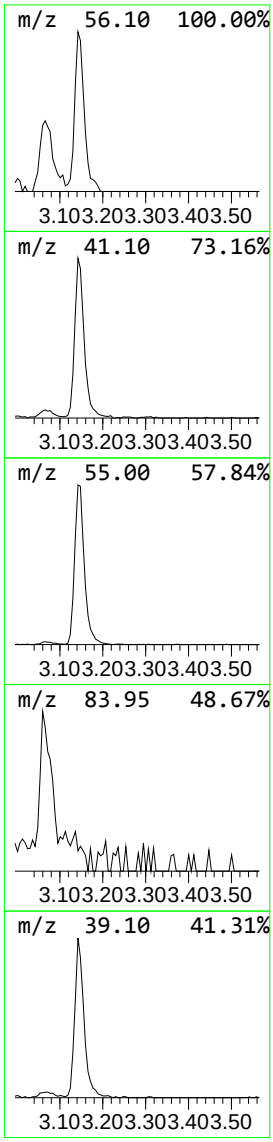
****

Peak Number 1 1-Pentene, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.066	3.61 ng	28298	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	50
3	Cyanic acid, 2-methylpropyl ester	99	C5H9NO	001768-25-8	47
4	1-Hexene	84	C6H12	000592-41-6	43
5	3-Buten-1-ol, 2-methyl-	86	C5H10O	004516-90-9	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051524\
Data File : BG061203.D
Acq On : 15 May 2024 12:56
Operator : MA/JU
Sample : P2450-01
Misc :
ALS Vial : 6 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

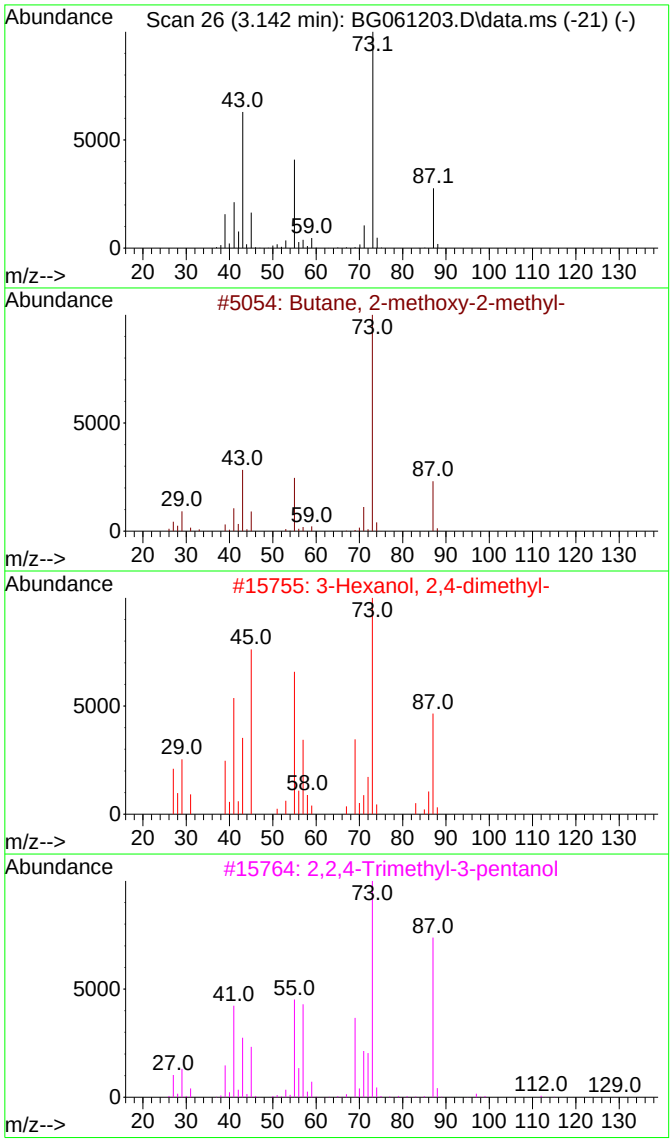
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

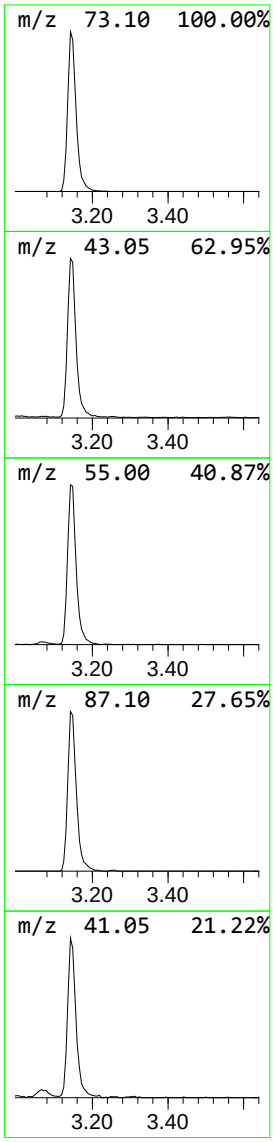
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.142	129.20 ng	1013110	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	3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	38
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
4	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	37
5	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	33





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051524\
Data File : BG061203.D
Acq On : 15 May 2024 12:56
Operator : MA/JU
Sample : P2450-01
Misc :
ALS Vial : 6 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

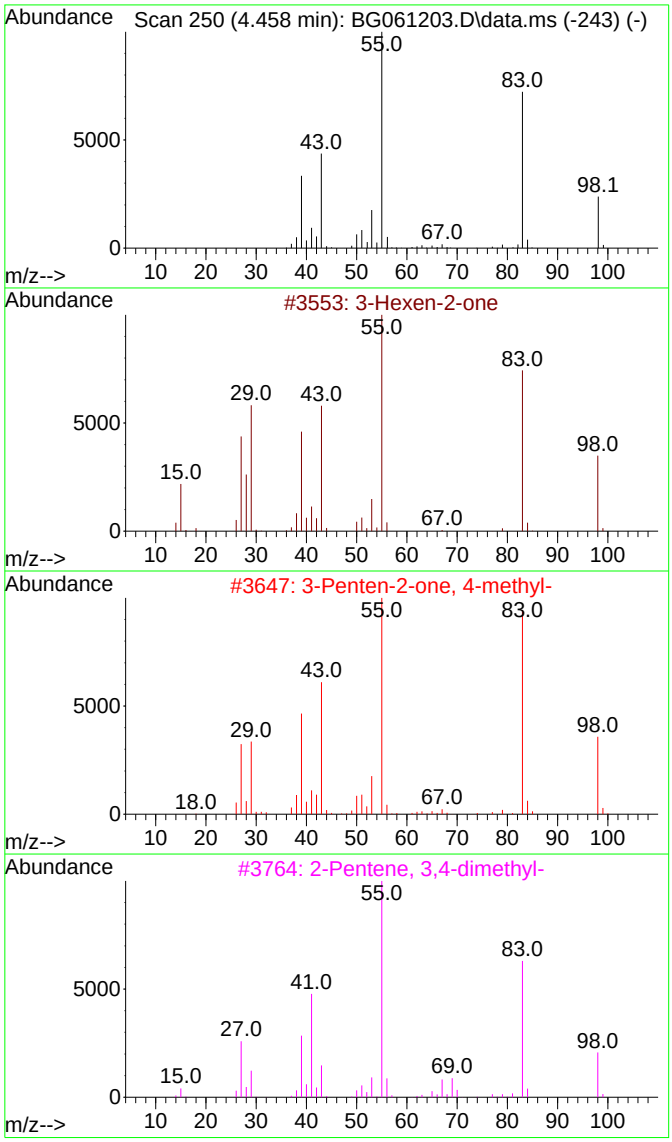
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

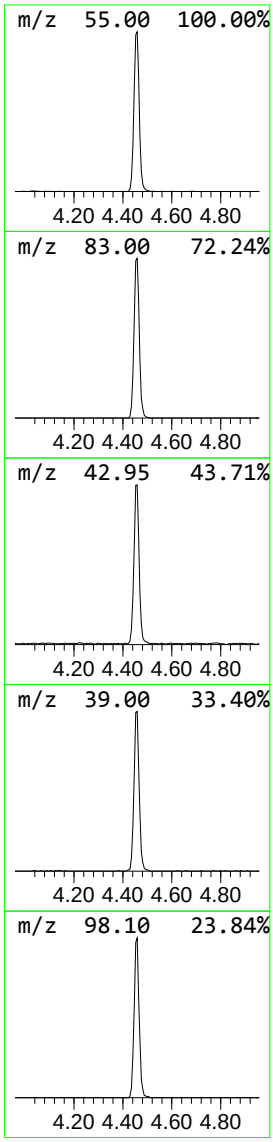
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.458	81.53 ng	639335	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	91
2	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	87
3	2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	78
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	72
5	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051524\
Data File : BG061203.D
Acq On : 15 May 2024 12:56
Operator : MA/JU
Sample : P2450-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1011UMR-RB240507-01

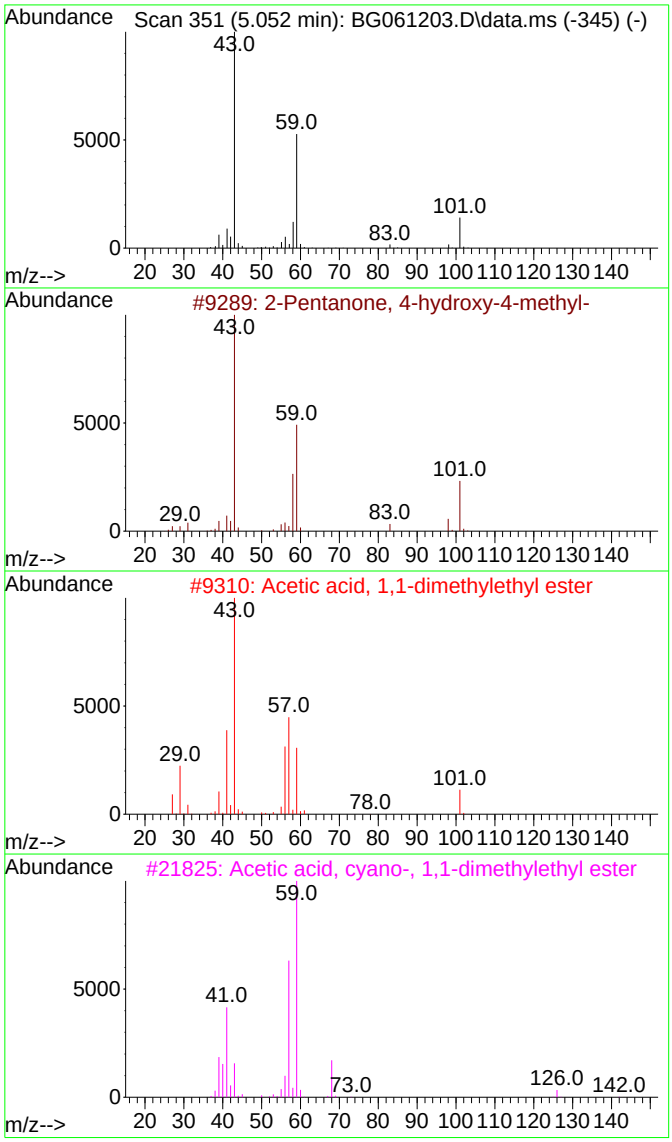
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

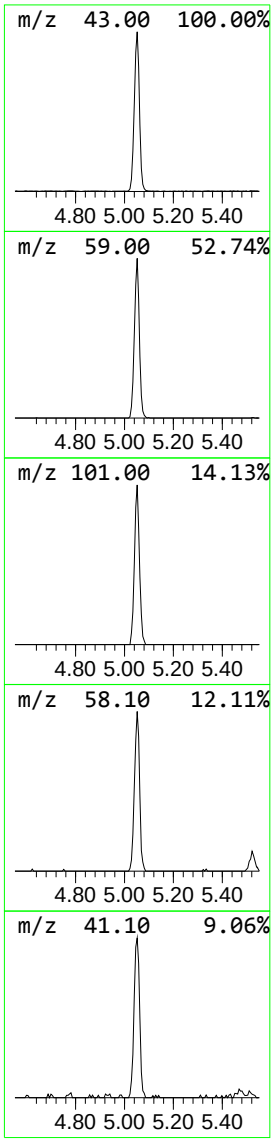
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.052	54.90 ng	430448	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	72
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051524\
Data File : BG061203.D
Acq On : 15 May 2024 12:56
Operator : MA/JU
Sample : P2450-01
Misc :
ALS Vial : 6 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

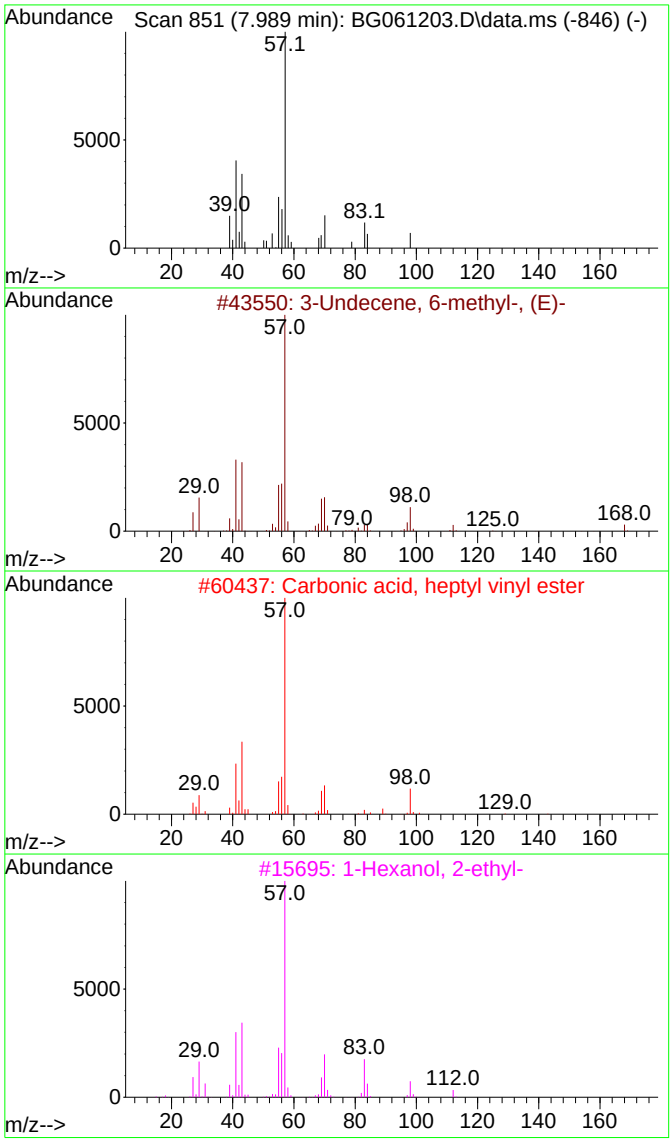
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

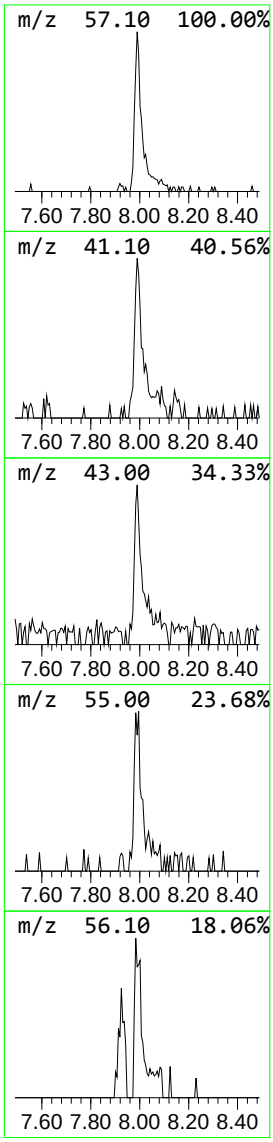
****

Peak Number 5 3-Undecene, 6-methyl-, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.989	4.53 ng	35488	1,4-Dichlorobenzene-d4	7.925

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Undecene, 6-methyl-, (E)-	168	C12H24	074630-52-7	59
2	Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	53
3	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	45
4	1-Hexene, 4-methyl-	98	C7H14	003769-23-1	43
5	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051524\
Data File : BG061203.D
Acq On : 15 May 2024 12:56
Operator : MA/JU
Sample : P2450-01
Misc :
ALS Vial : 6 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

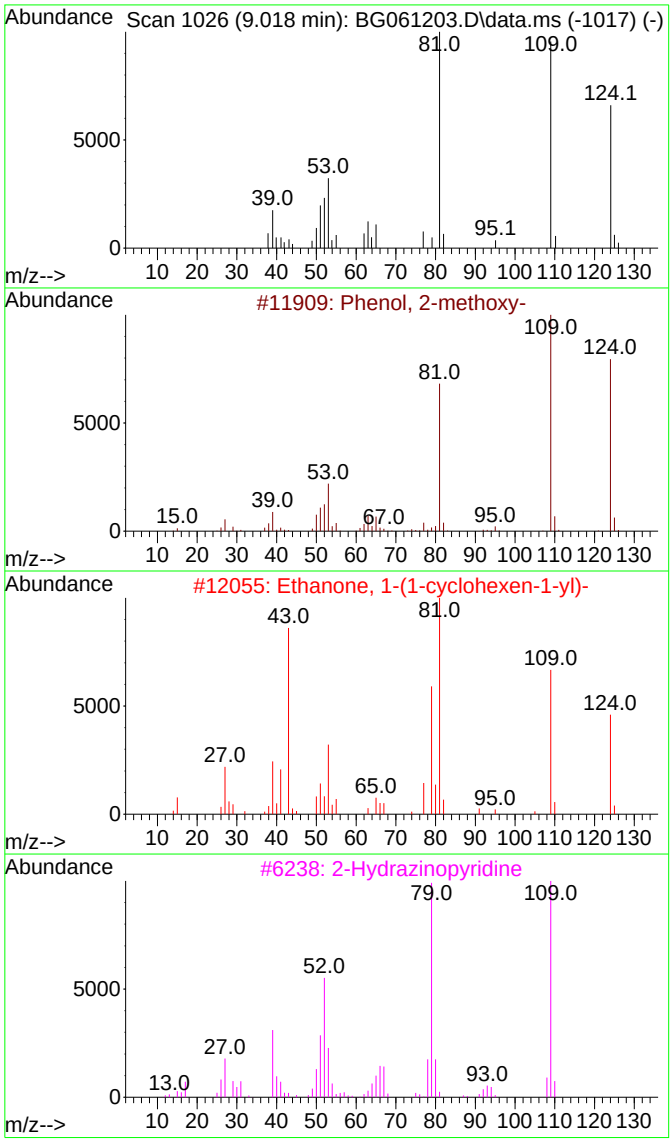
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

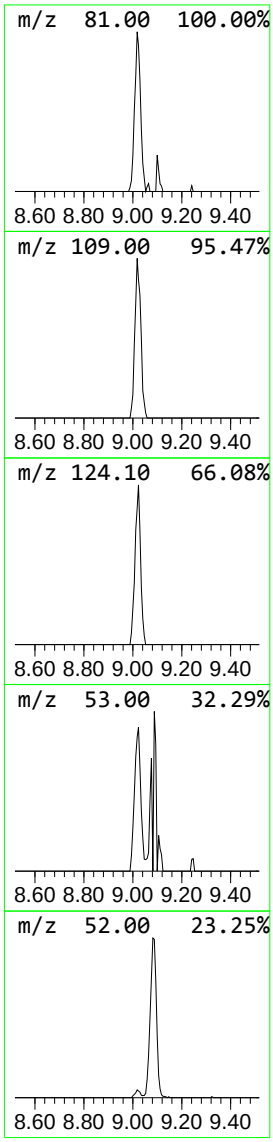
****

Peak Number 6 Phenol, 2-methoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.018	6.68 ng	52406	1,4-Dichlorobenzene-d4	7.925

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	96
2	Ethanone, 1-(1-cyclohexen-1-yl)-	124	C8H12O	000932-66-1	76
3	2-Hydrazinopyridine	109	C5H7N3	004930-98-7	46
4	Mequinol	124	C7H8O2	000150-76-5	46
5	Phenol, 4-amino-	109	C6H7NO	000123-30-8	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051524\
Data File : BG061203.D
Acq On : 15 May 2024 12:56
Operator : MA/JU
Sample : P2450-01
Misc :
ALS Vial : 6 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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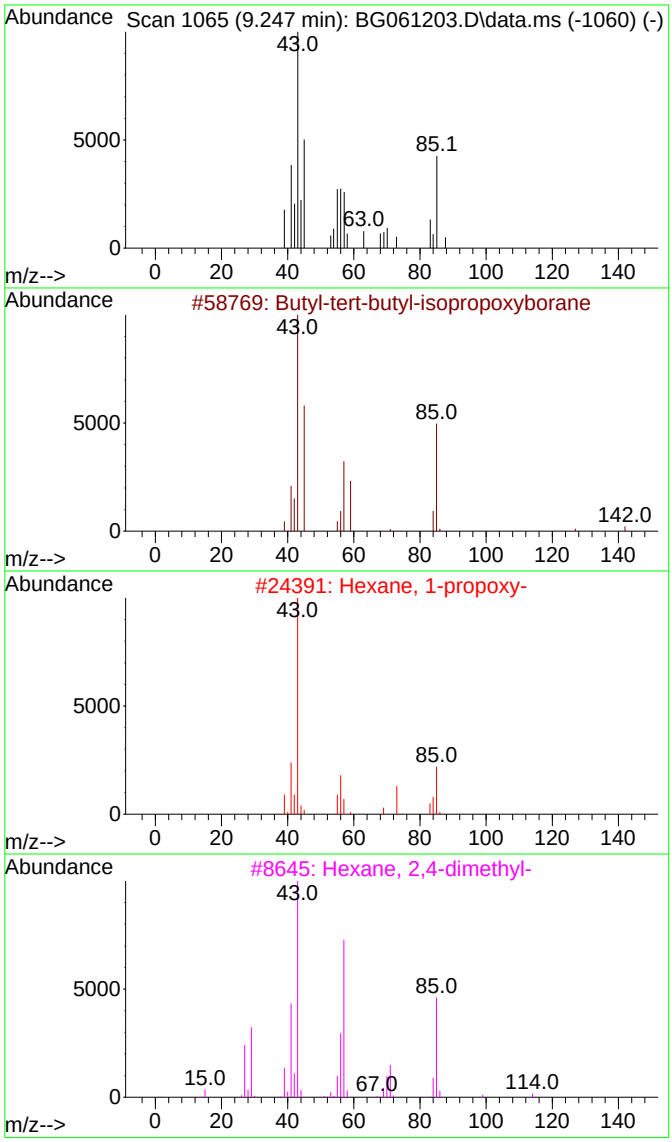
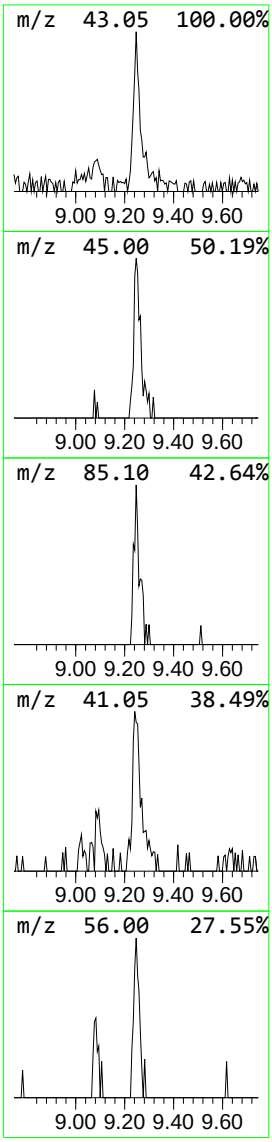
Peak Number 7 unknown9.247 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.247	3.08 ng	24117	1,4-Dichlorobenzene-d4	7.925

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl-tert-butyl-isopropoxyborane	184	C11H25BO	097782-82-6	38
2	Hexane, 1-propoxy-	144	C9H20O	053685-78-2	25
3	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	25
4	Heptane, 2,3-dimethyl-	128	C9H20	003074-71-3	17
5	2-Pentanone, 5,5'-oxybis-	186	C10H18O3	093677-66-8	16





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051524\
Data File : BG061203.D
Acq On : 15 May 2024 12:56
Operator : MA/JU
Sample : P2450-01
Misc :
ALS Vial : 6 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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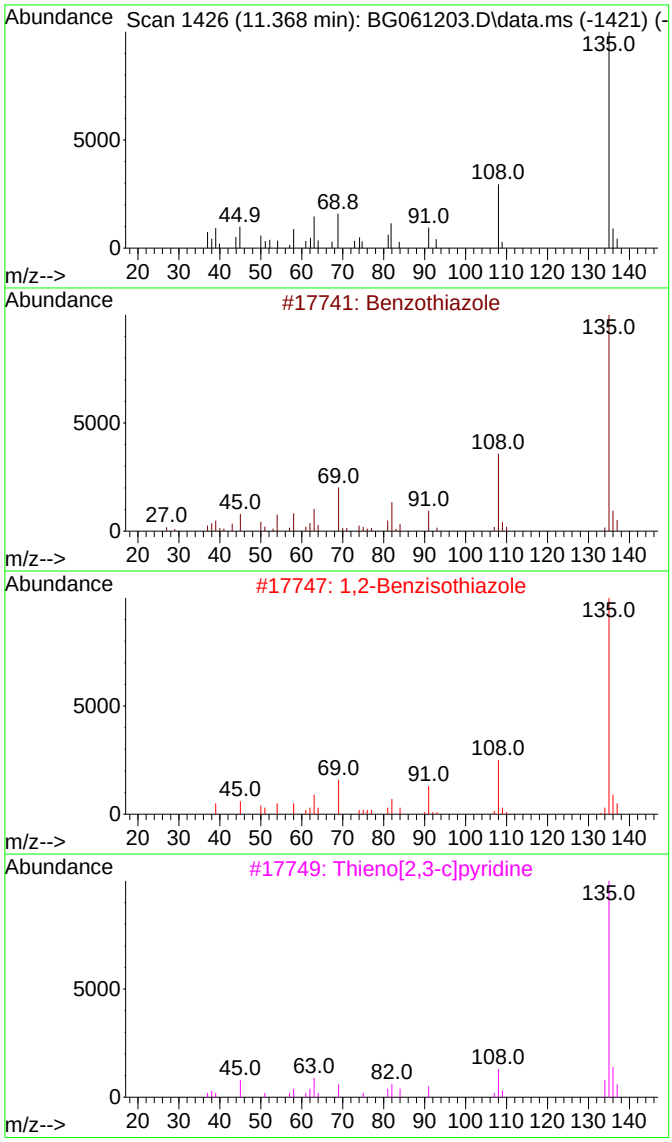
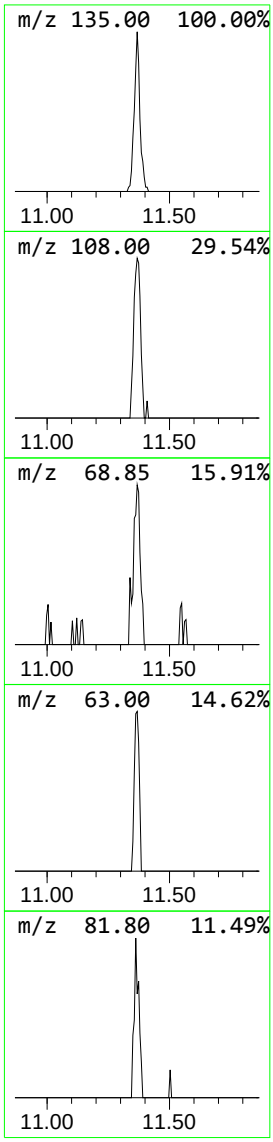
Peak Number 8 Benzothiazole Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.368	2.69 ng	28888	Naphthalene-d8	10.721

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzothiazole	135	C7H5NS	000095-16-9	91
2	1,2-Benzisothiazole	135	C7H5NS	000272-16-2	90
3	Thieno[2,3-c]pyridine	135	C7H5NS	000272-12-8	86
4	Thieno[3,2-c]pyridine	135	C7H5NS	000272-14-0	74
5	1H-Pyrazolo[3,4-d]pyrimidin-4-amine	135	C5H5N5	002380-63-4	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051524\
Data File : BG061203.D
Acq On : 15 May 2024 12:56
Operator : MA/JU
Sample : P2450-01
Misc :
ALS Vial : 6 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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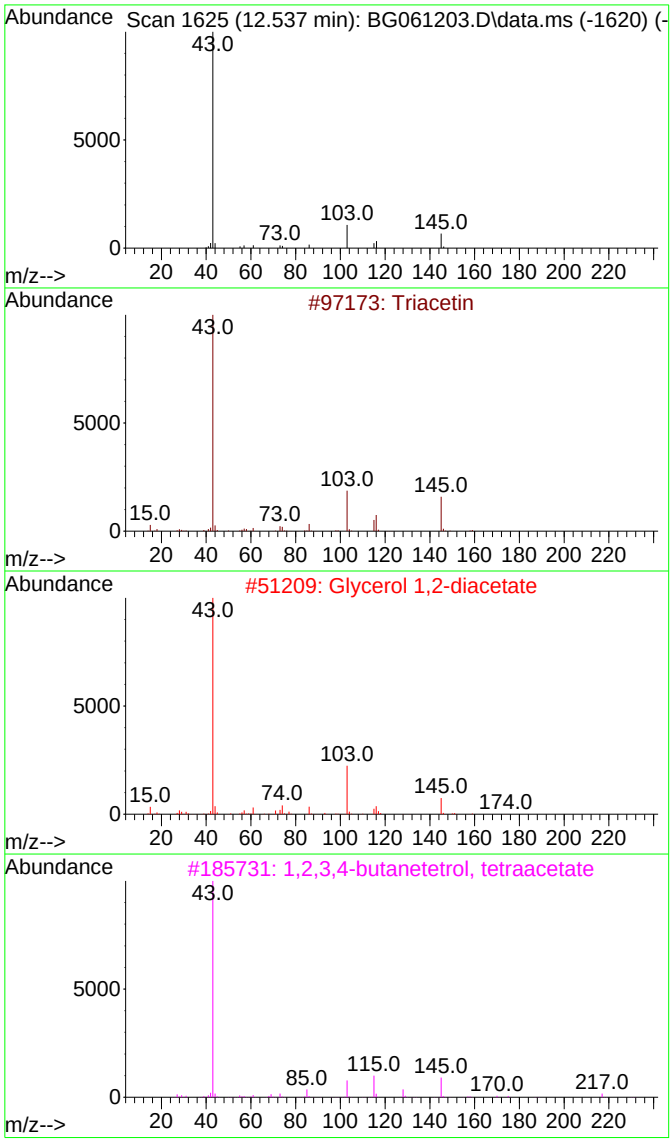
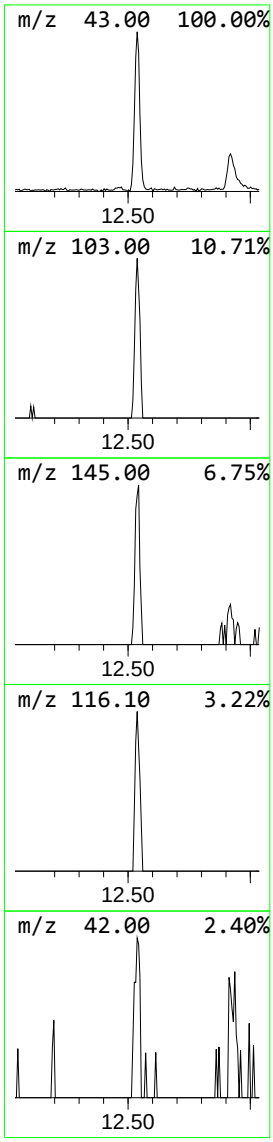
Peak Number 9 Triacetin Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.537	4.26 ng	45788	Naphthalene-d8	10.721

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacetin	218	C9H14O6	000102-76-1	83
2	Glycerol 1,2-diacetate	176	C7H12O5	000102-62-5	42
3	1,2,3,4-butanetetrol, tetraacetate	290	C12H18O8	073977-54-5	39
4	2-Deoxy-D-ribose, aldononitrile,...	257	C11H15NO6	1000380-43-1	39
5	Propanoic acid, 2-oxo-, ethyl ester	116	C5H8O3	000617-35-6	32





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Data File : BG061203.D
Acq On : 15 May 2024 12:56
Operator : MA/JU
Sample : P2450-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1011UMR-RB240507-01

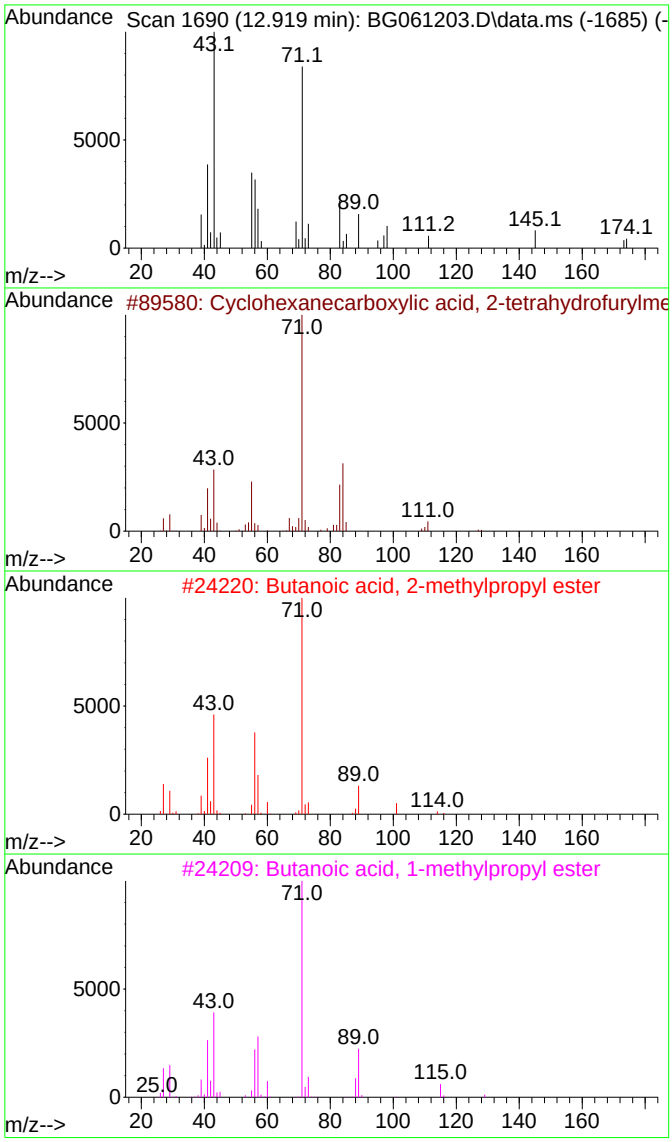
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

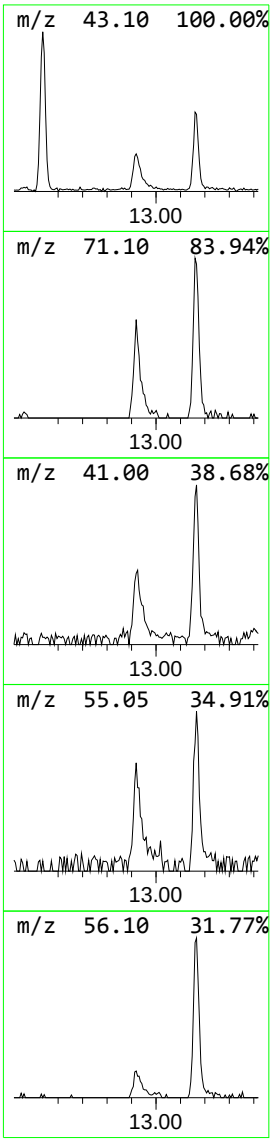
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Cyclohexanecarboxylic acid,... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.919	3.38 ng	51696	Acenaphthene-d10	14.558

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanecarboxylic acid, 2-te...	212	C12H20O3	1000279-85-7	50
2	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	40
3	Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	40
4	10-Undecenoic acid, 3-methylbuty...	254	C16H30O2	010214-27-4	38
5	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051524\
Data File : BG061203.D
Acq On : 15 May 2024 12:56
Operator : MA/JU
Sample : P2450-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1011UMR-RB240507-01

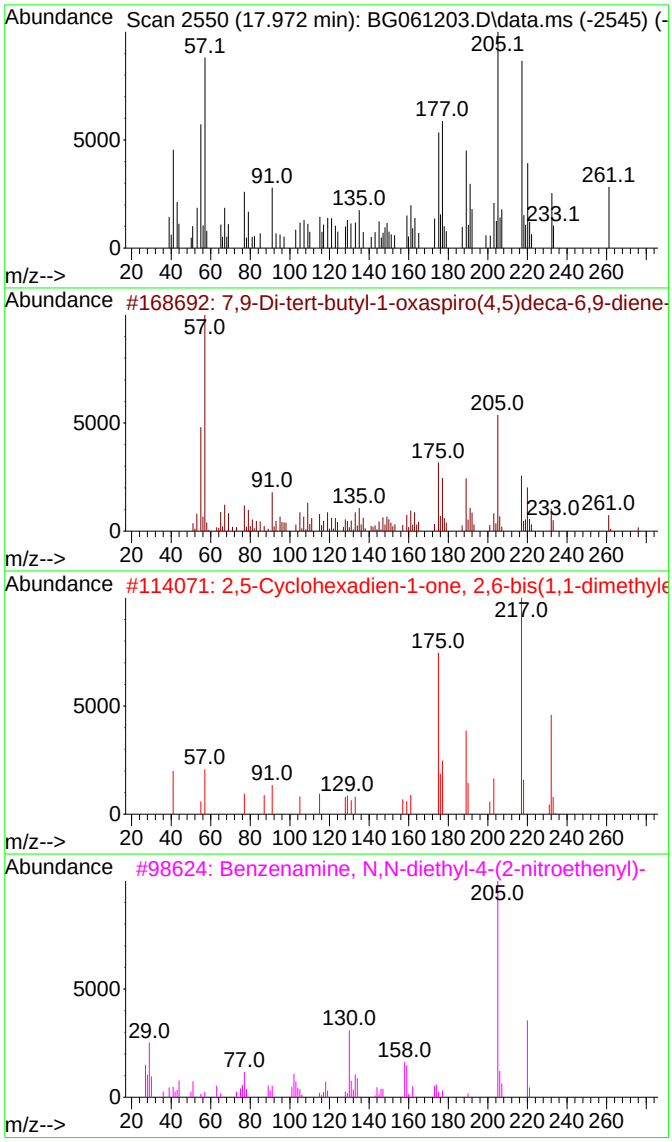
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

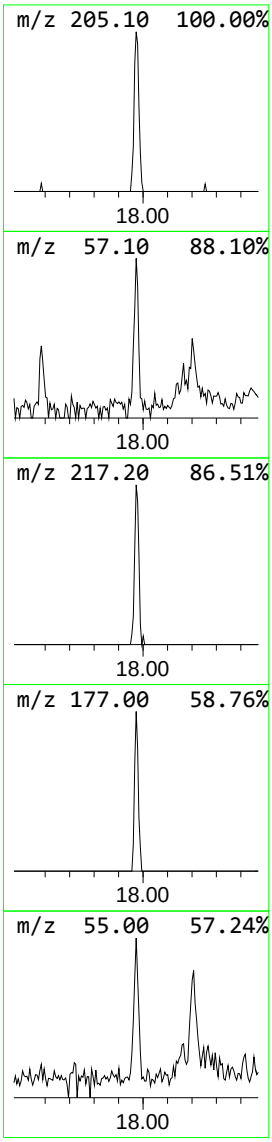
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.972	2.99 ng	57559	Phenanthrene-d10	17.308

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	83
2	2,5-Cyclohexadien-1-one, 2,6-bis...	232	C16H24O	006738-27-8	46
3	Benzenamine, N,N-diethyl-4-(2-ni...	220	C12H16N2O2	064462-51-7	38
4	(1R,3aR,5aR,9aS)-1,4,4,7-Tetrame...	220	C15H24O	104188-25-2	38
5	Xylazine	220	C12H16N2S	007361-61-7	38





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Data File : BG061203.D
Acq On : 15 May 2024 12:56
Operator : MA/JU
Sample : P2450-01
Misc :
ALS Vial : 6 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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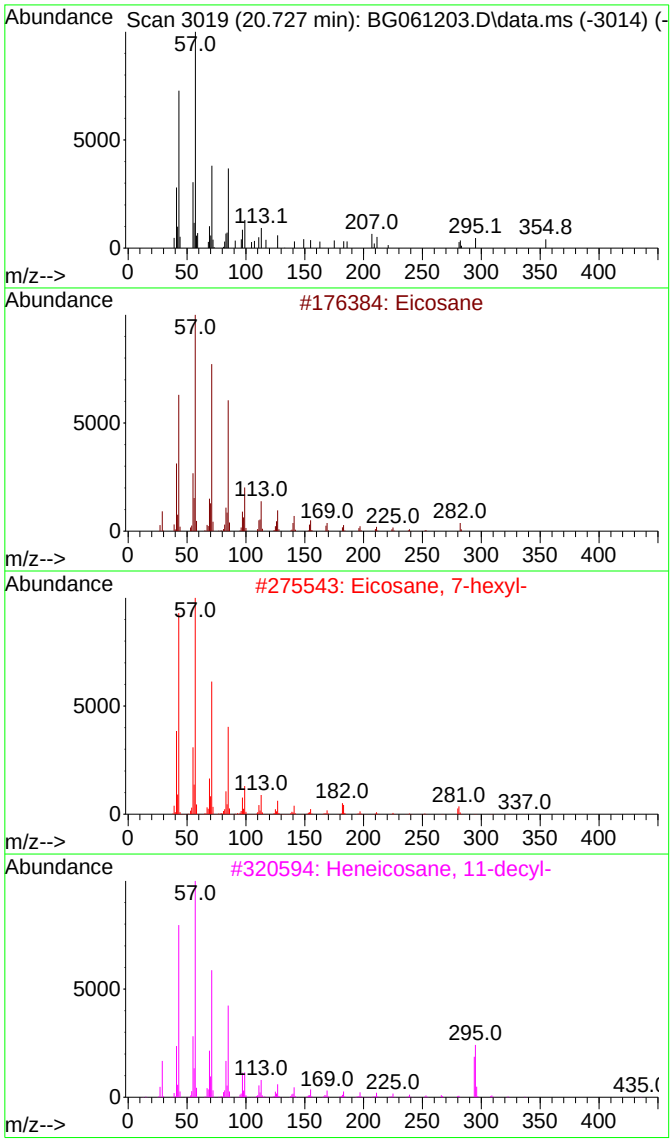
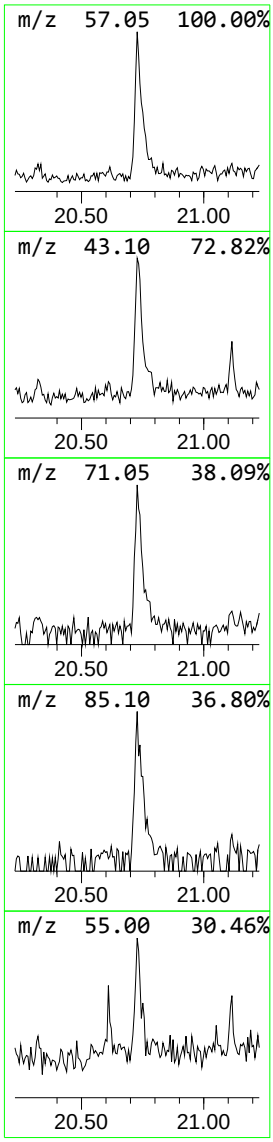
Peak Number 12 Eicosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.727	2.54 ng	58025	Chrysene-d12	21.567

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	68
2	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	68
3	Heneicosane, 11-decyl-	437	C31H64	055320-06-4	64
4	Dodecane, 4,9-dipropyl-	254	C18H38	003054-63-5	64
5	Docosane, 11-butyl-	366	C26H54	013475-76-8	62





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051524\
Data File : BG061203.D
Acq On : 15 May 2024 12:56
Operator : MA/JU
Sample : P2450-01
Misc :
ALS Vial : 6 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

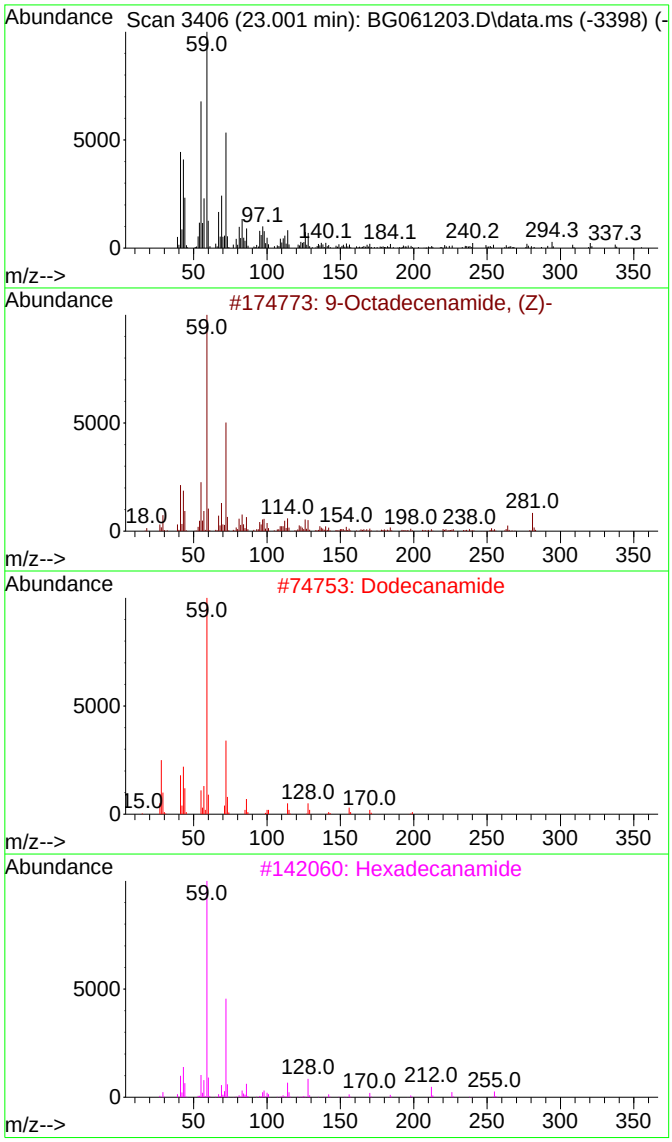
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

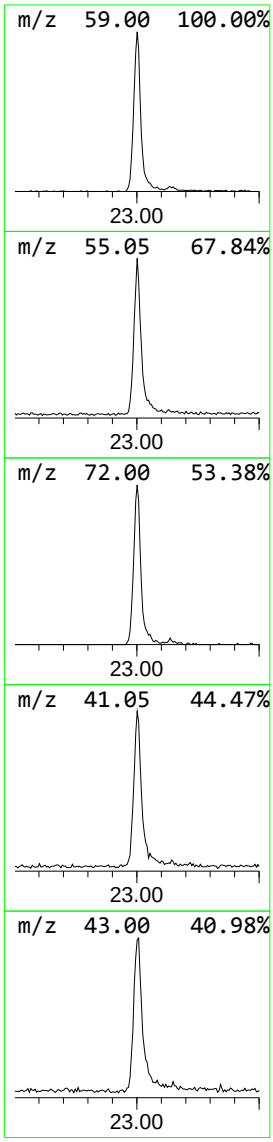
****

Peak Number 13 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.001	31.53 ng	719236	Chrysene-d12	21.567

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	74
2	Dodecanamide	199	C12H25NO	001120-16-7	74
3	Hexadecanamide	255	C16H33NO	000629-54-9	72
4	Octadecanamide	283	C18H37NO	000124-26-5	64
5	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	52





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051524\
Data File : BG061203.D
Acq On : 15 May 2024 12:56
Operator : MA/JU
Sample : P2450-01
Misc :
ALS Vial : 6 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	3.6	ng	28298	1	7.925	156825	20.0
Butane, 2-metho...	3.142	129.2	ng	1013110	1	7.925	156825	20.0
3-Hexen-2-one	4.458	81.5	ng	639335	1	7.925	156825	20.0
2-Pentanone, 4-...	5.052	54.9	ng	430448	1	7.925	156825	20.0
3-Undecene, 6-m...	7.989	4.5	ng	35488	1	7.925	156825	20.0
Phenol, 2-methoxy-	9.018	6.7	ng	52406	1	7.925	156825	20.0
unknown9.247	9.247	3.1	ng	24117	1	7.925	156825	20.0
Benzothiazole	11.368	2.7	ng	28888	2	10.721	215000	20.0
Triacetin	12.537	4.3	ng	45788	2	10.721	215000	20.0
Cyclohexanecarb...	12.919	3.4	ng	51696	3	14.558	305871	20.0
7,9-Di-tert-but...	17.972	3.0	ng	57559	4	17.308	384415	20.0
Eicosane	20.727	2.5	ng	58025	5	21.567	456182	20.0
9-Octadecenamid...	23.001	31.5	ng	719236	5	21.567	456182	20.0