LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051624\
Data File : BG061223.D
Acq On : 16 May 2024 16:39
Operator : MA/JU
Sample : P2476-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-1-COMP

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: BG061223.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.076	9	15	22	rVV4	9434	20751	1.09%	0.218%
2	3.146	22	27	42	rVB	290148	462849	24.25%	4.870%
3	3.669	111	116	127	rBV	44054	66109	3.46%	0.696%
4	5.526	425	432	441	rBV	431522	685763	35.94%	7.215%
5	7.106	694	701	716	rBV	453685	792636	41.54%	8.340%
6	7.929	834	841	848	rBV	94702	156206	8.19%	1.644%
7	9.080	1029	1037	1045	rBV	285267	510869	26.77%	5.375%
8	10.490	1270	1277	1285	rBV2	47448	82381	4.32%	0.867%
9	10.720	1308	1316	1324	rBV	123604	222858	11.68%	2.345%
10	11.460	1435	1442	1448	rBV2	14850	26211	1.37%	0.276%
11	13.176	1727	1734	1744	rBV	749813	1168334	61.22%	12.293%
12	14.556	1963	1969	1978	rVB	214682	334602	17.53%	3.521%
13	14.756	1998	2003	2004	rBV	17342	21928	1.15%	0.231%
14	14.774	2004	2006	2012	rVB3	21754	26733	1.40%	0.281%
15	16.049	2217	2223	2237	rBV	701306	1125632	58.99%	11.843%
16	17.306	2430	2437	2442	rBV	289950	440451	23.08%	4.634%
17	17.688	2496	2502	2506	rBV6	11525	23137	1.21%	0.243%
18	18.205	2585	2590	2598	rBV5	29478	49716	2.61%	0.523%
19	19.357	2782	2786	2790	rBV	27942	40923	2.14%	0.431%
20	19.721	2845	2848	2855	rVB2	22577	38403	2.01%	0.404%
21	19.926	2877	2883	2890	rBV	1417888	1908286	100.00%	20.078%
22	20.608	2995	2999	3007	rVB	70408	91968	4.82%	0.968%
23	21.225	3100	3104	3115	rBV4	32952	66538	3.49%	0.700%
24	21.566	3155	3162	3167	rBV	302114	524162	27.47%	5.515%
25	22.541	3323	3328	3335	rVB3	43301	90025	4.72%	0.947%
26	24.680	3684	3692	3704	rVB2	182636	526777	27.60%	5.543%

Sum of corrected areas: 9504248

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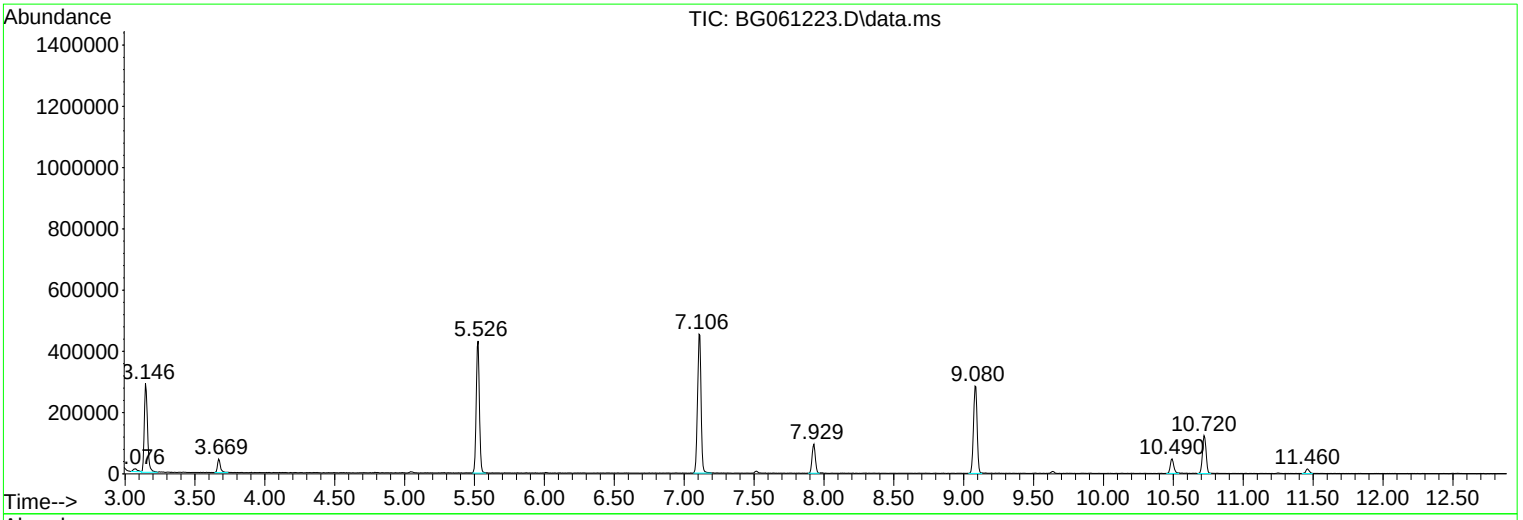
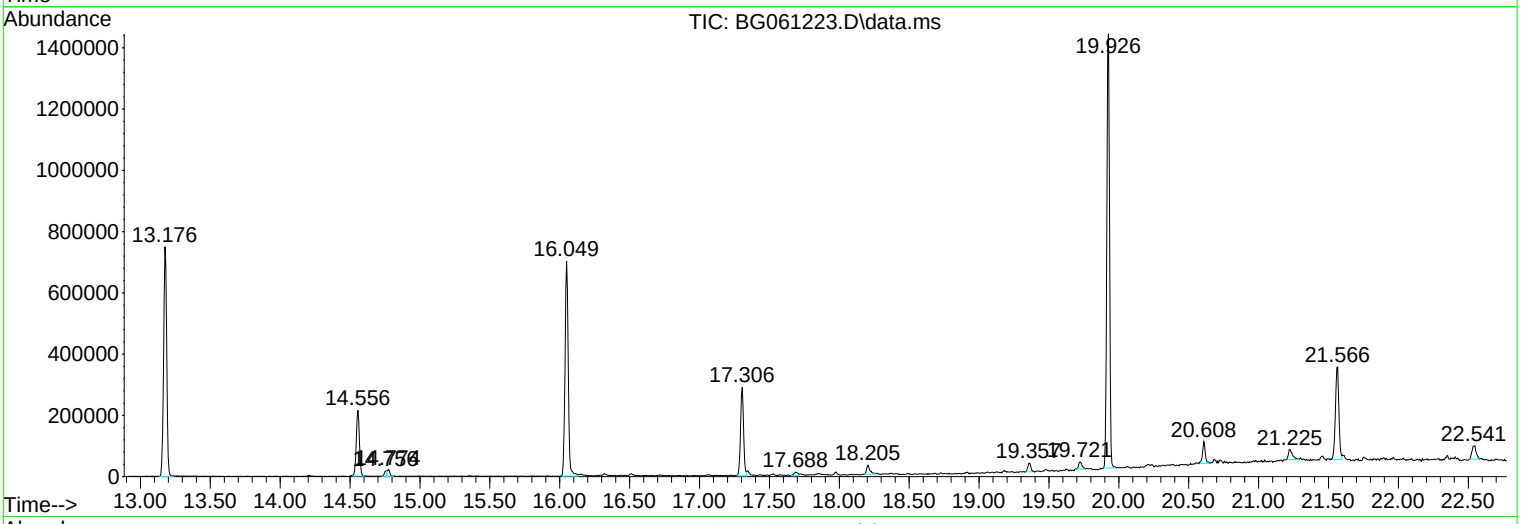
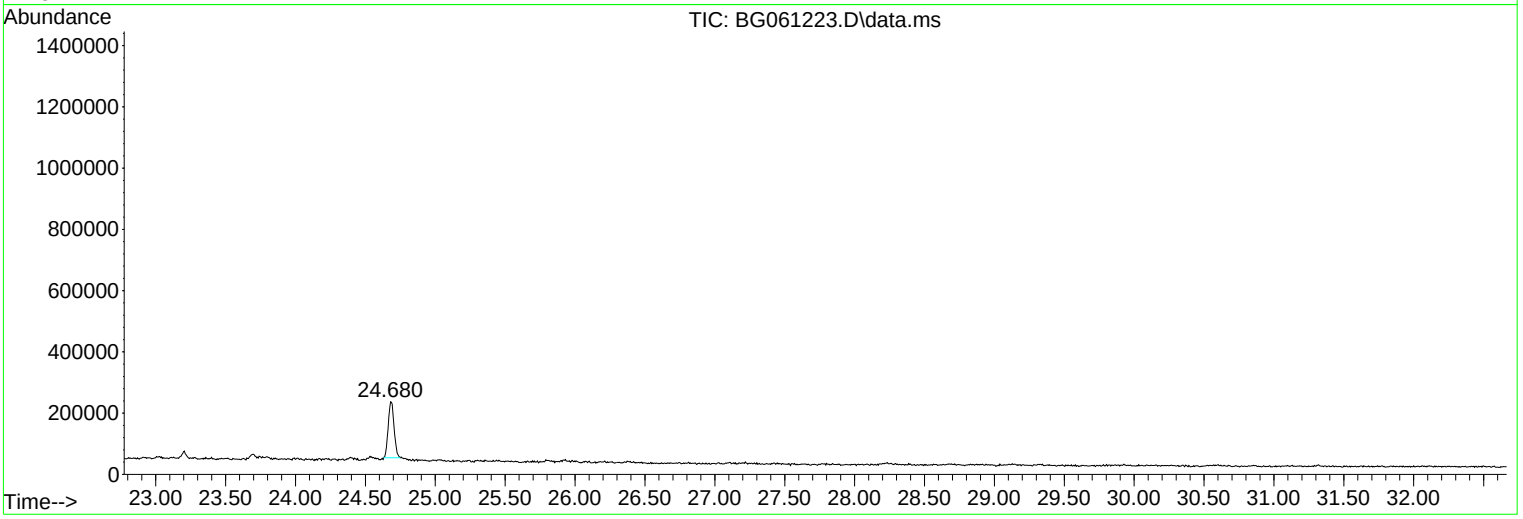
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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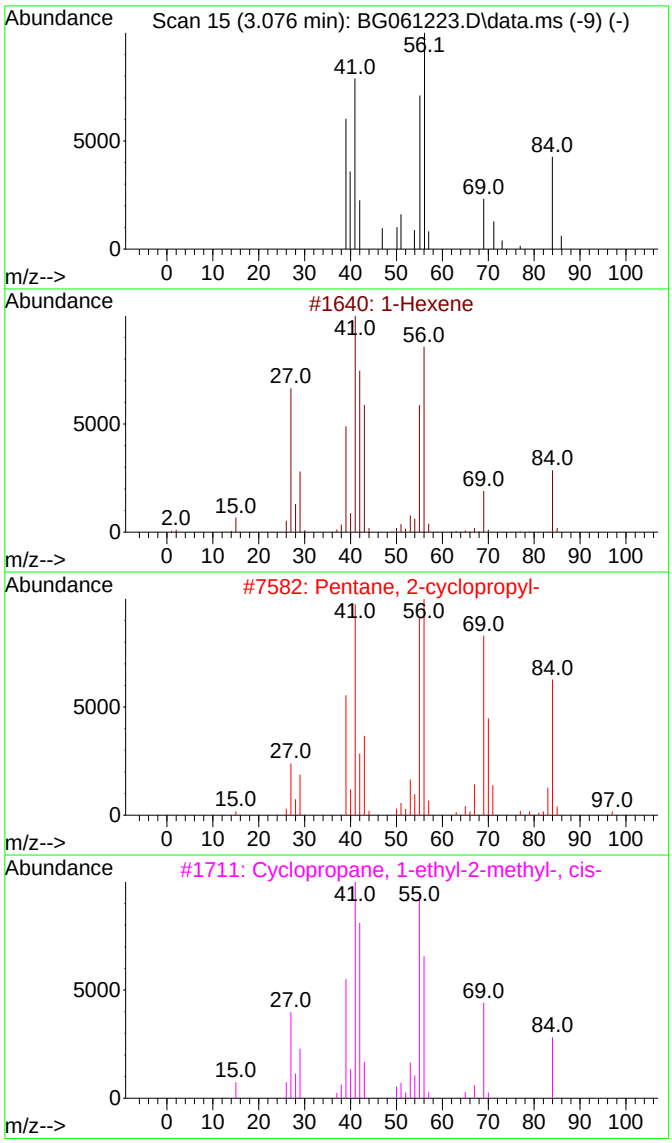
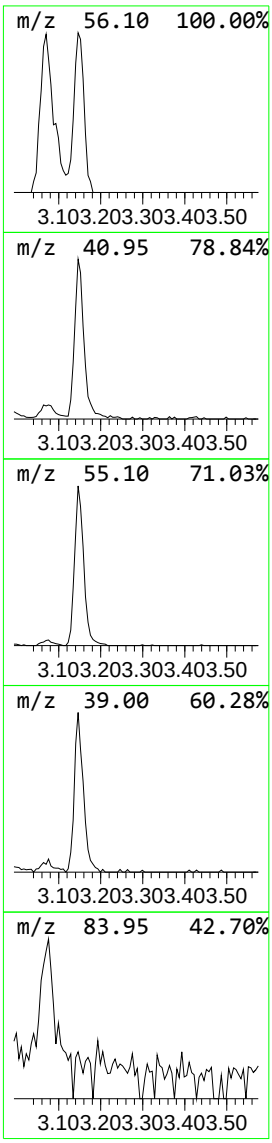
****

Peak Number 1 1-Hexene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.076	2.66 ng	20751	1,4-Dichlorobenzene-d4	7.929

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexene	84	C6H12	000592-41-6	59
2	Pentane, 2-cyclopropyl-	112	C8H16	005458-16-2	45
3	Cyclopropane, 1-ethyl-2-methyl-,...	84	C6H12	019781-68-1	42
4	Oxirane, (1-methylbutyl)-	114	C7H14O	053229-39-3	40
5	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	38





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Operator : MA/JU
Sample : P2476-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-1-COMP

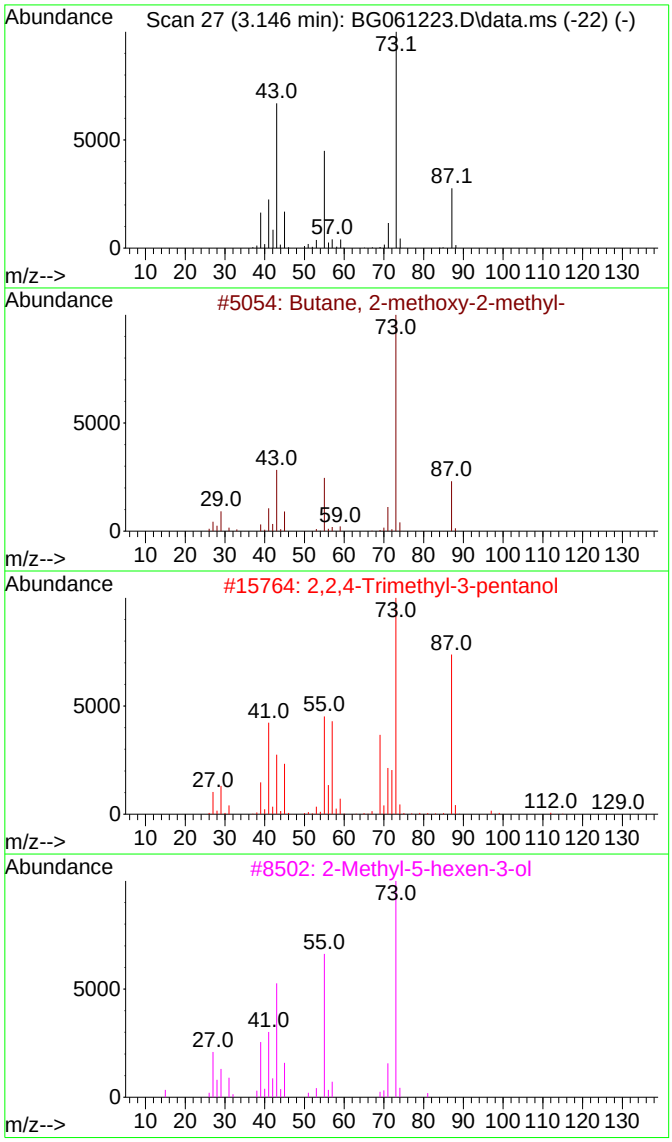
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

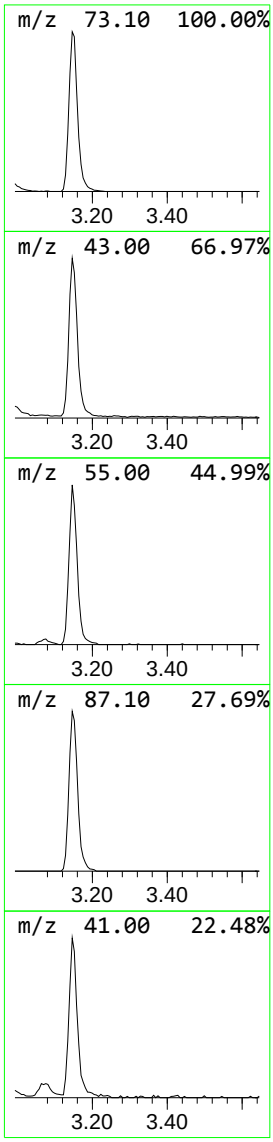
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.146	59.26 ng	462849	1,4-Dichlorobenzene-d4	7.929

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	33
4	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	33
5	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	25





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Sample : P2476-01
Misc :
ALS Vial : 9 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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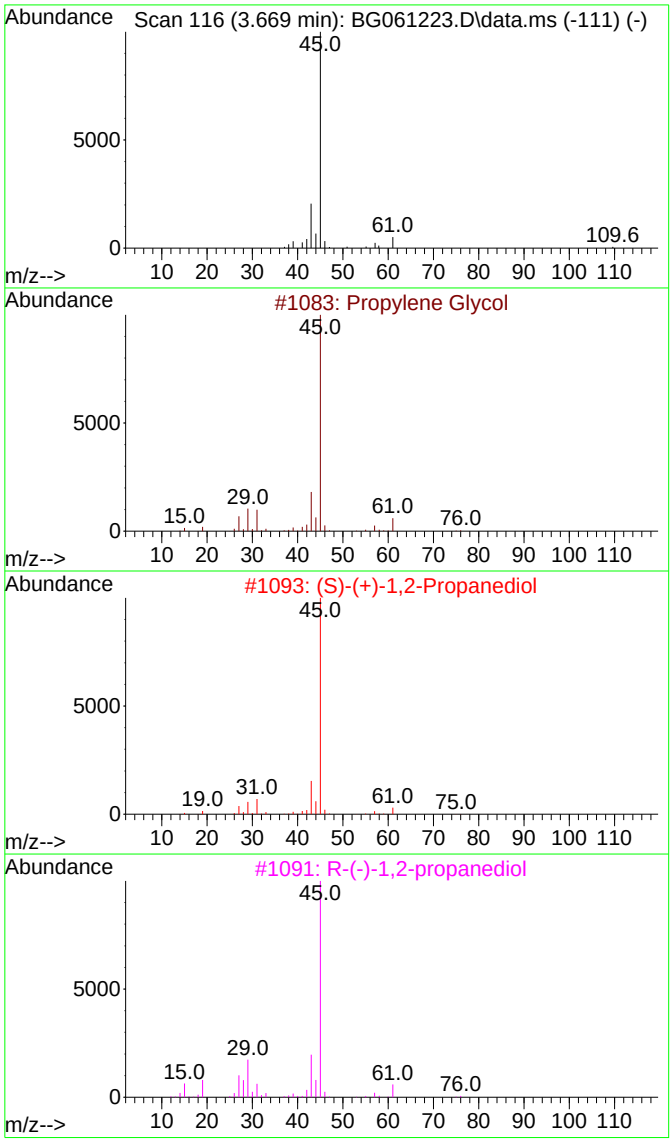
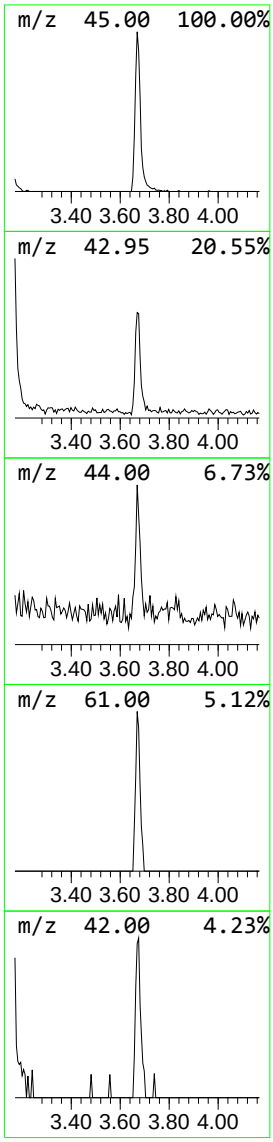
****

Peak Number 3 unknown3.669 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.669	8.46 ng	66109	1,4-Dichlorobenzene-d4	7.929

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	43
2	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	43
3	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
4	3-Ethyl-2-pentanol	116	C7H16O	000609-27-8	40
5	2-Heptanol, (S)-	116	C7H16O	006033-23-4	9





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Operator : MA/JU
Sample : P2476-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-1-COMP

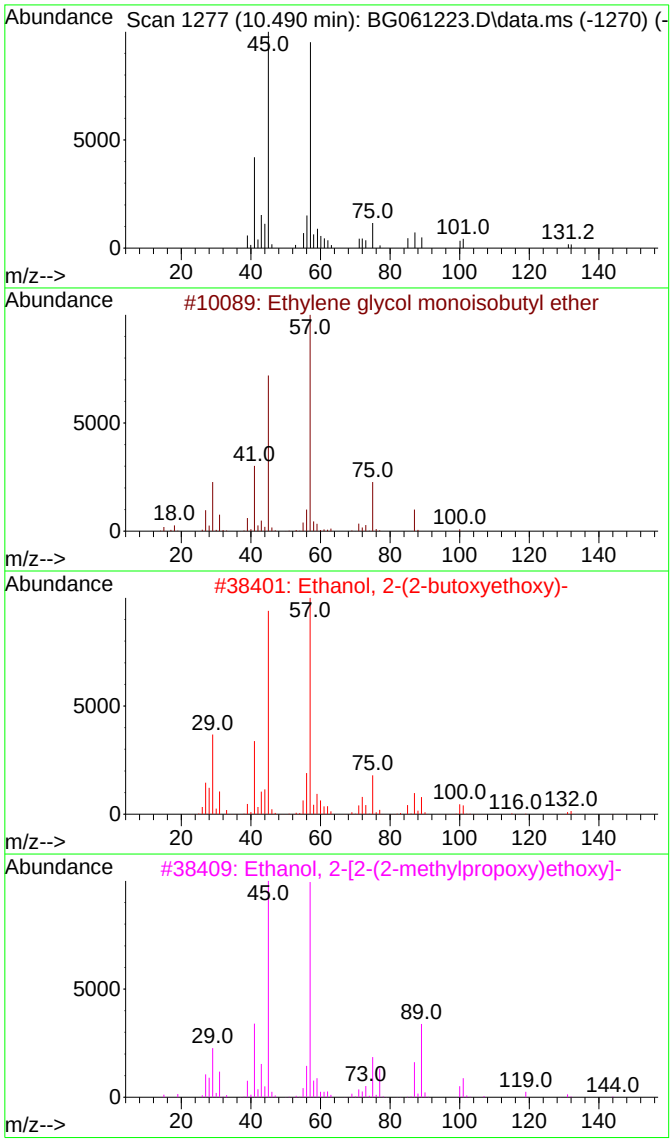
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

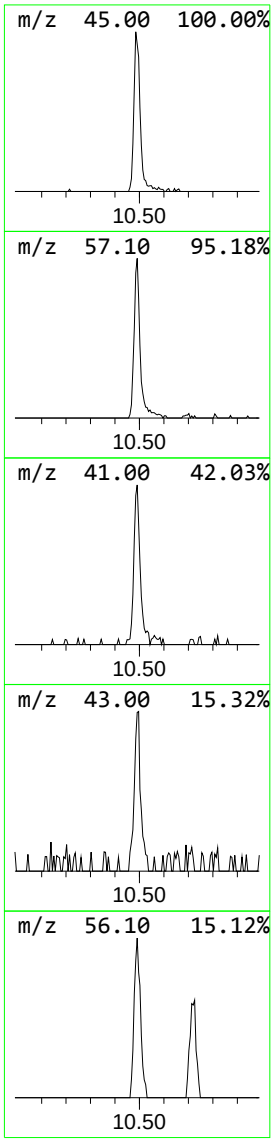
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Ethylene glycol monoisobuty... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.491	7.39 ng	82381	Naphthalene-d8	10.720

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
2	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	50
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
4	2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	45
5	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	42





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Sample : P2476-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
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TIC Library : C:\Database\NIST20.L
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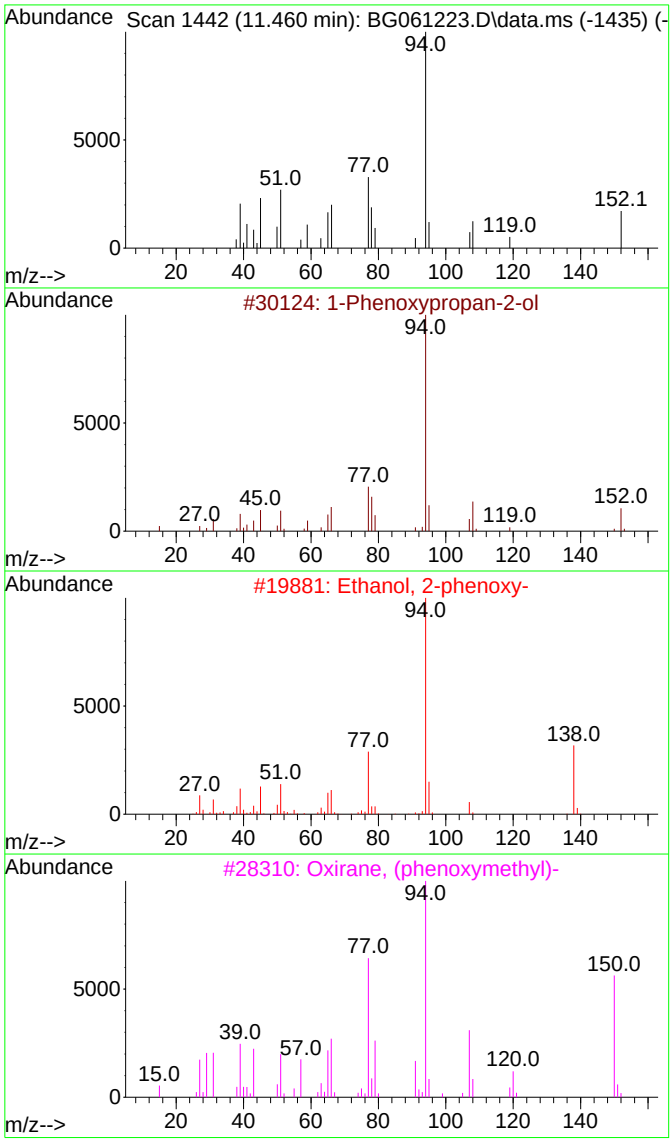
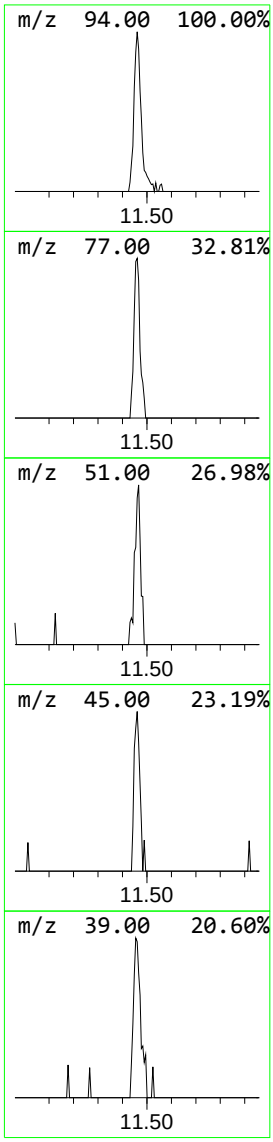
****

Peak Number 5 1-Phenoxypropan-2-ol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.460	2.35 ng	26211	Naphthalene-d8	10.720

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	94
2	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	72
3	Oxirane, (phenoxymethyl)-	150	C9H10O2	000122-60-1	53
4	Phenol	94	C6H6O	000108-95-2	50
5	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	47





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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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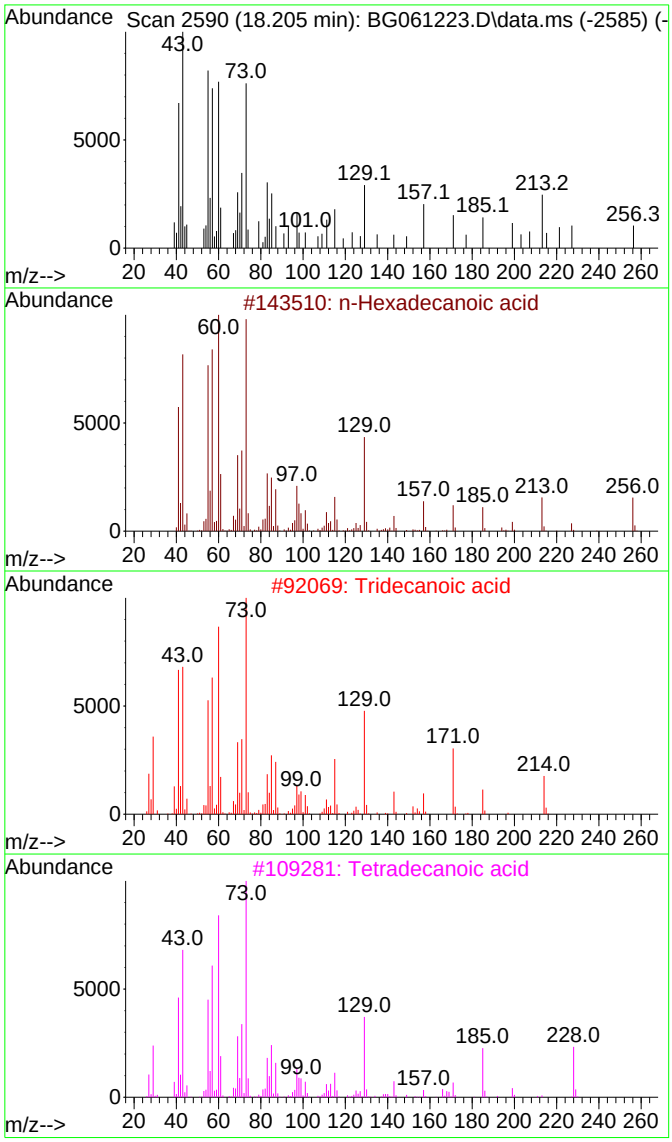
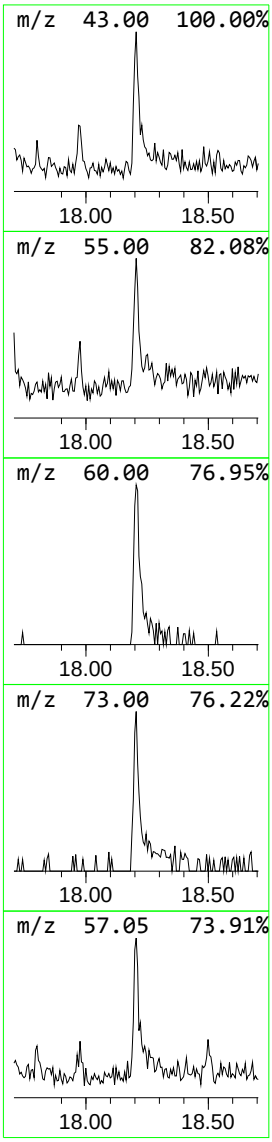
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.205	2.26 ng	49716	Phenanthrene-d10	17.306

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
2	Tridecanoic acid	214	C13H26O2	000638-53-9	50
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	47
4	Dodecanoic acid	200	C12H24O2	000143-07-7	47
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	47





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Operator : MA/JU
Sample : P2476-01
Misc :
ALS Vial : 9 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

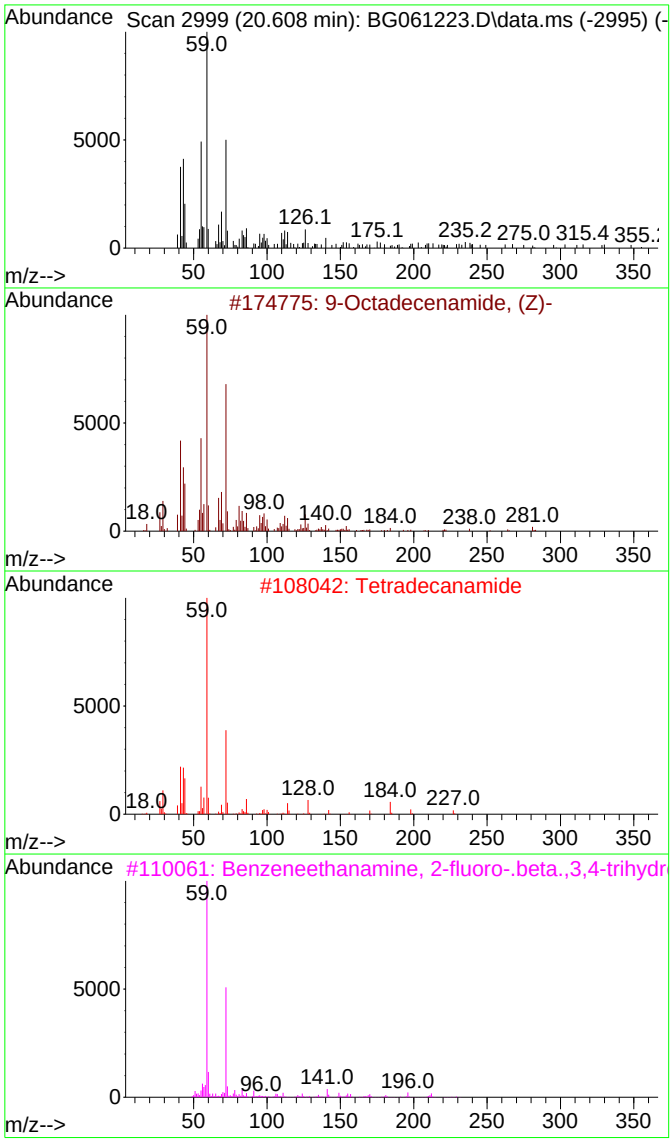
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

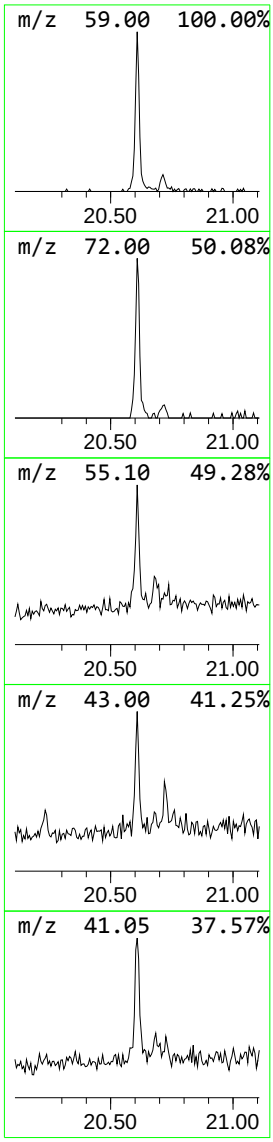
****

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.608	3.51 ng	91968	Chrysene-d12	21.560

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	95
2	Tetradecanamide	227	C14H29NO	000638-58-4	78
3	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	64
4	Palmitoleamide	253	C16H31NO	106010-22-4	64
5	Nonanamide	157	C9H19NO	001120-07-6	59





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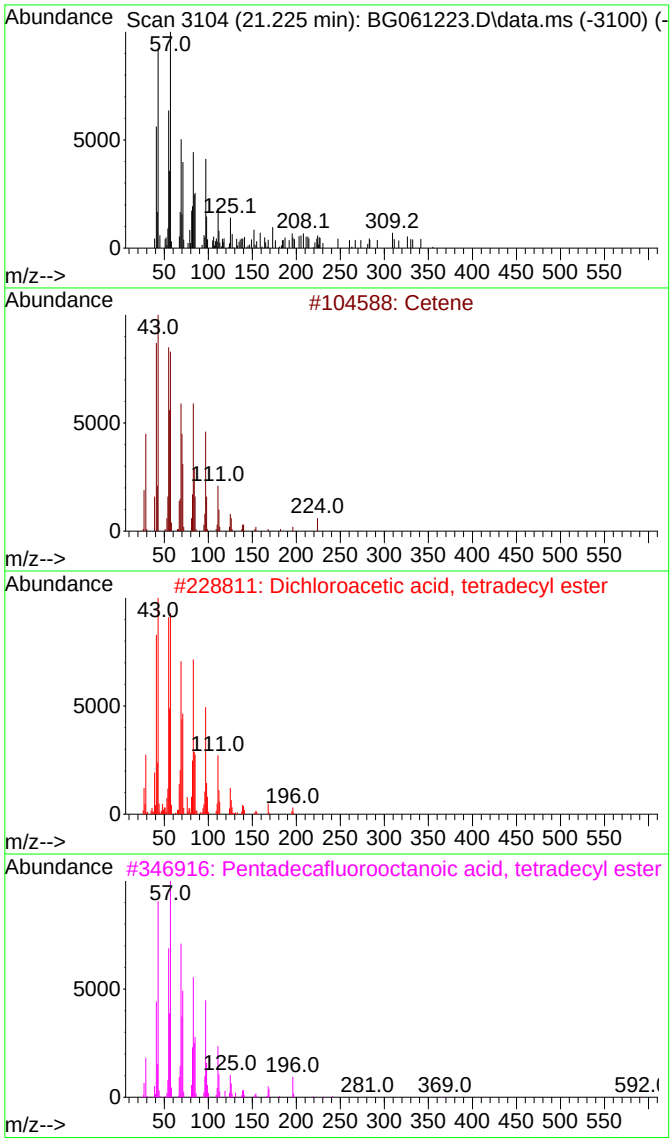
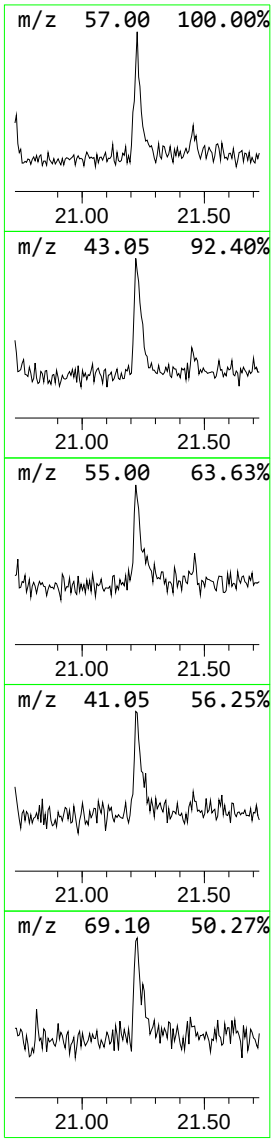
****

Peak Number 8 Cetene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.225	2.54 ng	66538	Chrysene-d12	21.560

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cetene	224	C16H32	000629-73-2	92
2	Dichloroacetic acid, tetradecyl ...	324	C16H30Cl2O2	083005-02-1	83
3	Pentadecafluorooctanoic acid, te...	610	C22H29F15O2	1000406-04-4	83
4	Dichloroacetic acid, 2-tetradecy...	324	C16H30Cl2O2	1000280-64-4	83
5	Trichloroacetic acid, tridecyl e...	344	C15H27Cl3O2	074339-51-8	81





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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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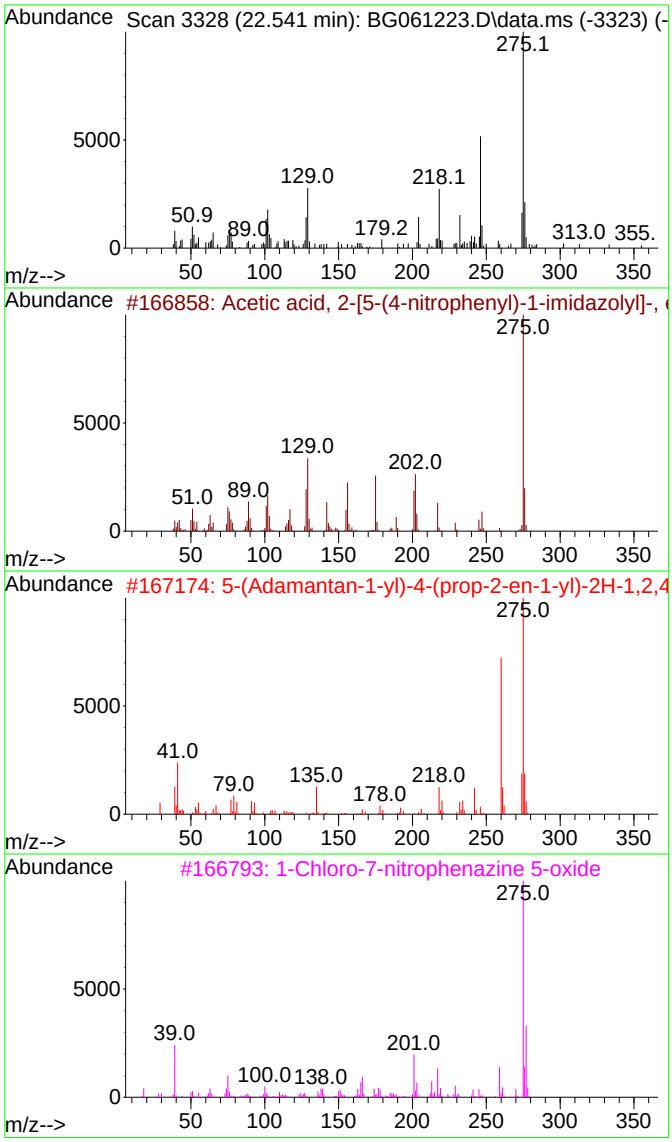
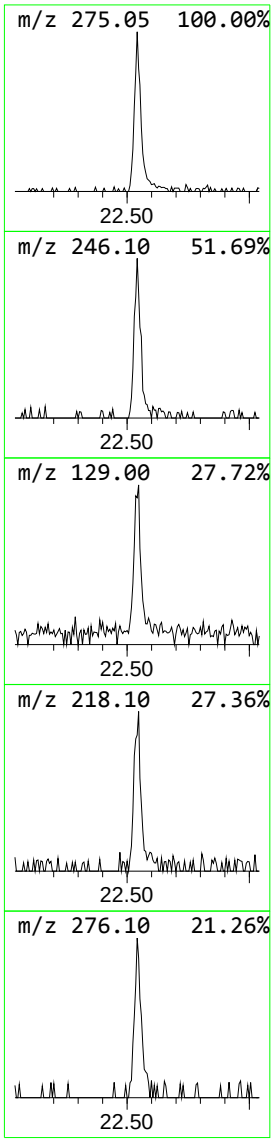
****
Peak Number 9 Acetic acid, 2-[5-(4-nitrop... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.541	3.44 ng	90025	Chrysene-d12	21.560

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, 2-[5-(4-nitrophenyl...	275	C13H13N3O4	351064-45-4	78
2	5-(Adamantan-1-yl)-4-(prop-2-en-...	275	C15H21N3S	345987-96-4	49
3	1-Chloro-7-nitrophenazine 5-oxide	275	C12H6ClN3O3	023663-48-1	38
4	3-Methyl-6-(4-nitro-phenyl)-7H-[...	275	C11H9N5O2S	1000296-64-4	38
5	Cyclohexanecarboxylic acid, 2-(2...	275	C16H21NO3	296246-15-6	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051624\
Data File : BG061223.D
Acq On : 16 May 2024 16:39
Operator : MA/JU
Sample : P2476-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-1-COMP

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-Hexene	3.076	2.7	ng	20751	1	7.929	156206	20.0
Butane, 2-metho...	3.146	59.3	ng	462849	1	7.929	156206	20.0
unknown3.669	3.669	8.5	ng	66109	1	7.929	156206	20.0
Ethylene glycol...	10.491	7.4	ng	82381	2	10.720	222858	20.0
1-Phenoxypropan...	11.460	2.4	ng	26211	2	10.720	222858	20.0
n-Hexadecanoic ...	18.205	2.3	ng	49716	4	17.306	440451	20.0
9-Octadecenamid...	20.608	3.5	ng	91968	5	21.560	524162	20.0
Cetene	21.225	2.5	ng	66538	5	21.560	524162	20.0
Acetic acid, 2-...	22.541	3.4	ng	90025	5	21.560	524162	20.0