LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048979.D
Acq On : 15 Jun 2021 15:57
Operator : CG/JU
Sample : M2672-19
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(80-84)

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-BG061121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048979.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.162	17	21	35	rVB	77588	141824	3.15%	0.777%
2	3.285	38	42	52	rVB	64233	97923	2.18%	0.536%
3	5.670	441	448	455	rBV	918938	1558867	34.66%	8.536%
4	7.274	711	721	732	rBV	1009020	1837560	40.85%	10.062%
5	8.115	857	864	872	rVB	140963	239452	5.32%	1.311%
6	9.284	1055	1063	1075	rBV	626004	1132798	25.19%	6.203%
7	10.700	1299	1304	1310	rBV2	26564	47482	1.06%	0.260%
8	10.941	1338	1345	1352	rBV	174548	323627	7.20%	1.772%
9	13.385	1752	1761	1768	rBV	1602774	2543321	56.55%	13.927%
10	14.760	1987	1995	2006	rBV	280699	455233	10.12%	2.493%
11	16.158	2228	2233	2239	rVB2	68780	93634	2.08%	0.513%
12	16.246	2241	2248	2265	rBV	1606416	2500071	55.58%	13.690%
13	17.509	2456	2463	2469	rBV	381787	578119	12.85%	3.166%
14	17.627	2478	2483	2489	rVB3	52461	73993	1.65%	0.405%
15	18.391	2608	2613	2621	rBV	150206	210061	4.67%	1.150%
16	19.660	2824	2829	2838	rBV3	113881	163123	3.63%	0.893%
17	20.118	2900	2907	2917	rVB	3418758	4497848	100.00%	24.630%
18	20.794	3017	3022	3031	rBV	58203	95512	2.12%	0.523%
19	20.876	3031	3036	3040	rVV	40099	51517	1.15%	0.282%
20	21.434	3126	3131	3136	rBV4	62395	114492	2.55%	0.627%
21	21.687	3170	3174	3180	rVB2	76025	108571	2.41%	0.595%
22	21.804	3187	3194	3201	rBV	376714	656408	14.59%	3.594%
23	23.026	3397	3402	3410	rVB5	42833	84740	1.88%	0.464%
24	25.142	3752	3762	3772	rBV2	212436	655756	14.58%	3.591%

Sum of corrected areas: 18261932

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
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Misc :
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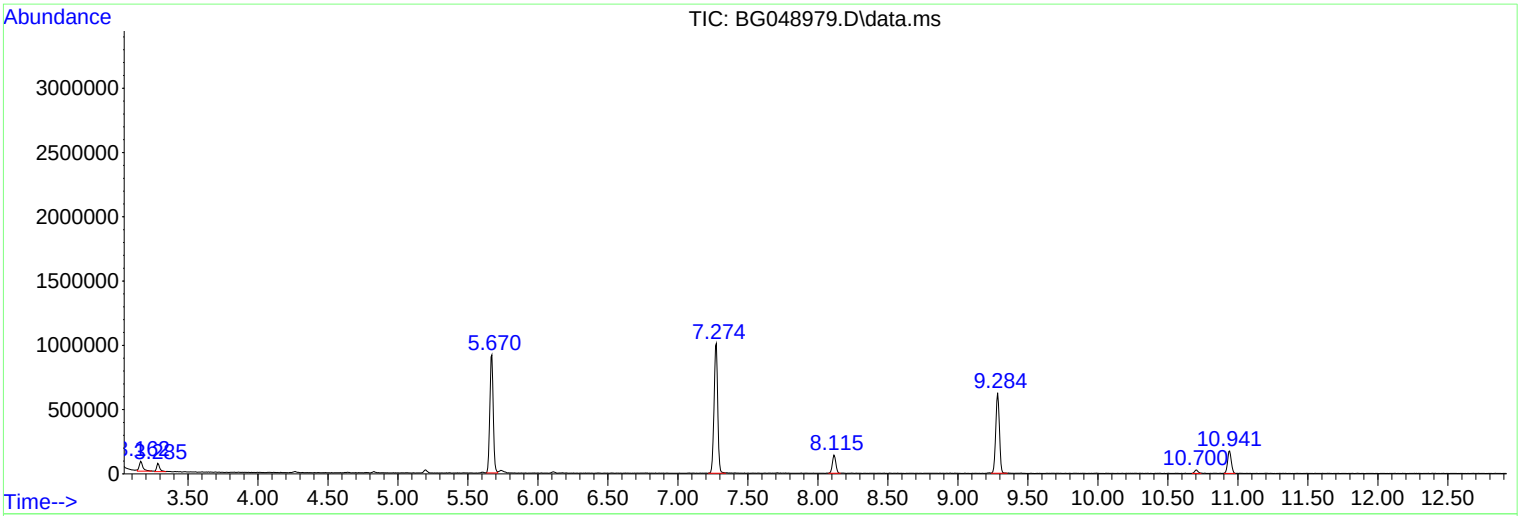
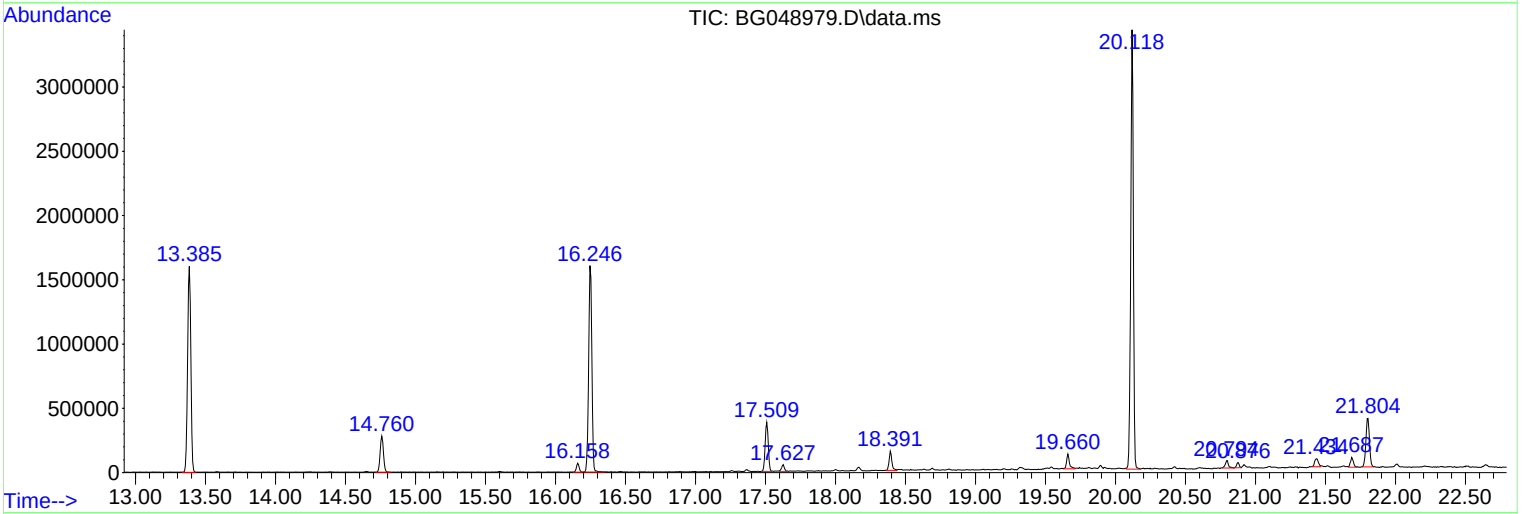
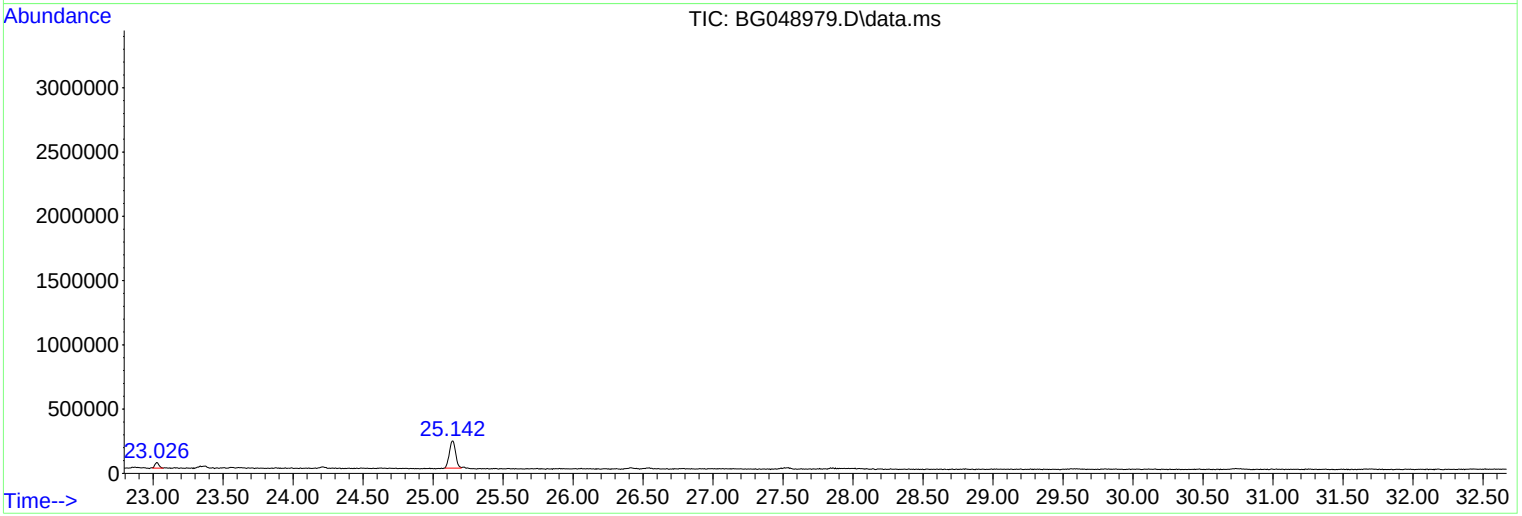
Instrument :
BNA_G
ClientSampleId :
17-B6(80-84)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P







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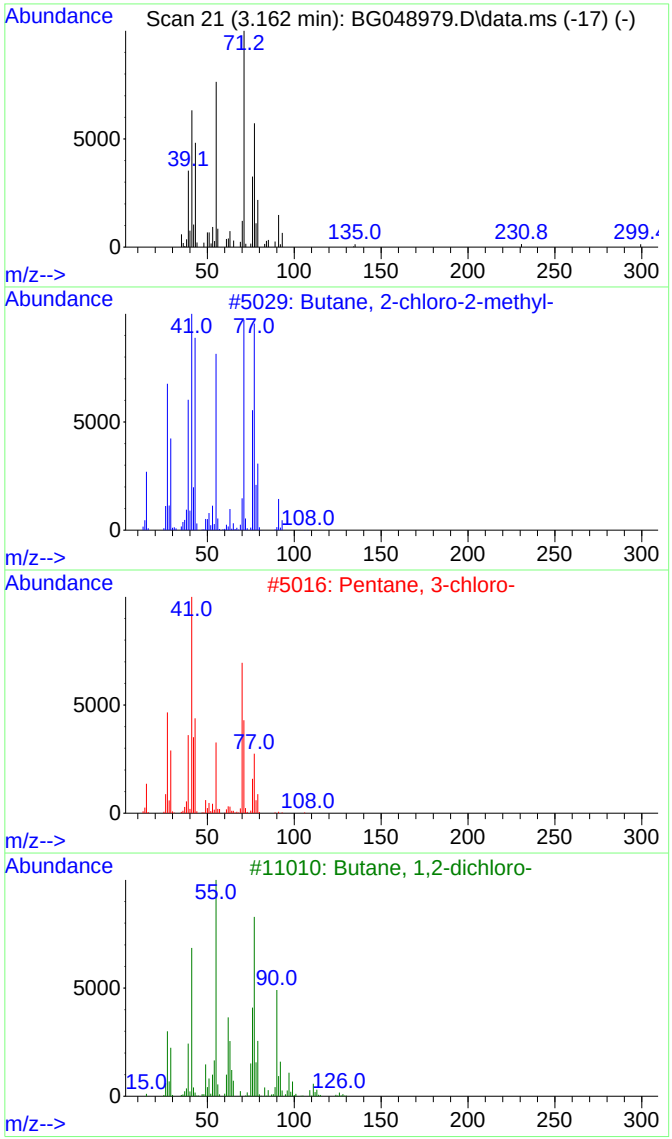
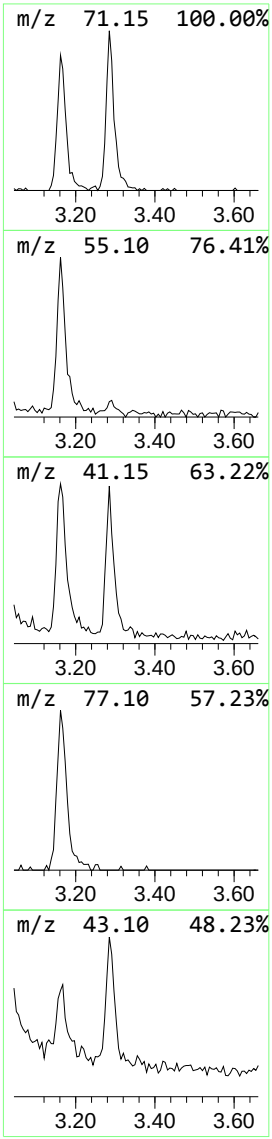
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.162	11.85 ng	141824	1,4-Dichlorobenzene-d4	8.115

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-chloro-2-methyl-	106	C5H11Cl	000594-36-5	50
2	Pentane, 3-chloro-	106	C5H11Cl	000616-20-6	39
3	Butane, 1,2-dichloro-	126	C4H8Cl2	000616-21-7	17
4	Propane, 1,1-dichloro-	112	C3H6Cl2	000078-99-9	16
5	2-Furanmethanamine, tetrahydro-	101	C5H11NO	004795-29-3	16





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Data File : BG048979.D
Acq On : 15 Jun 2021 15:57
Operator : CG/JU
Sample : M2672-19
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(80-84)

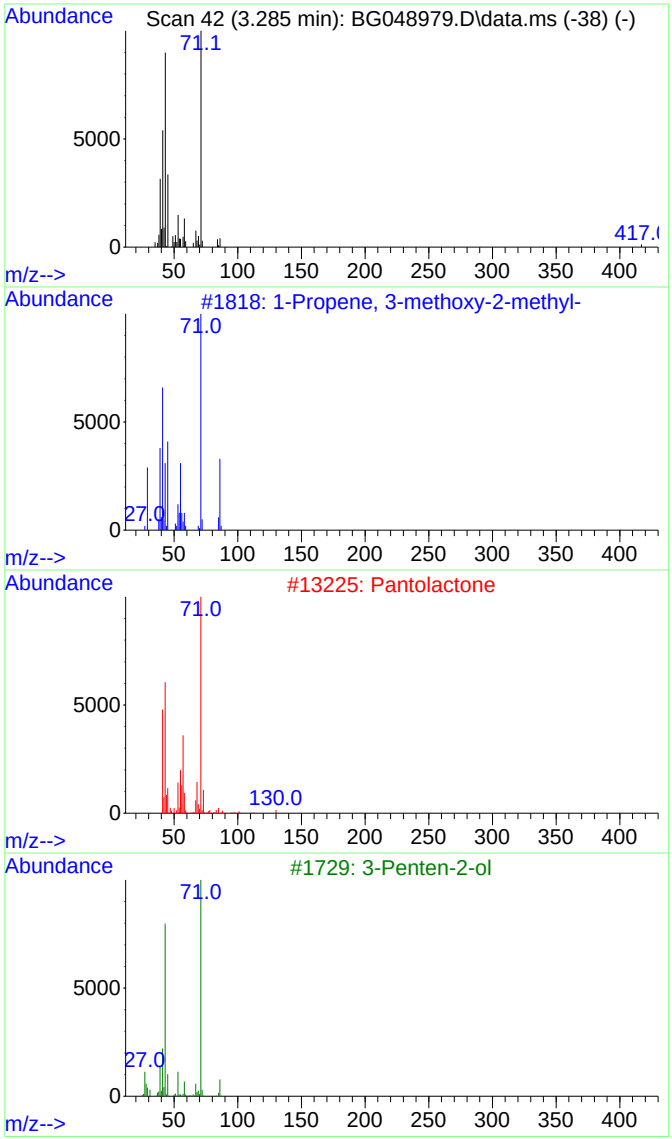
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

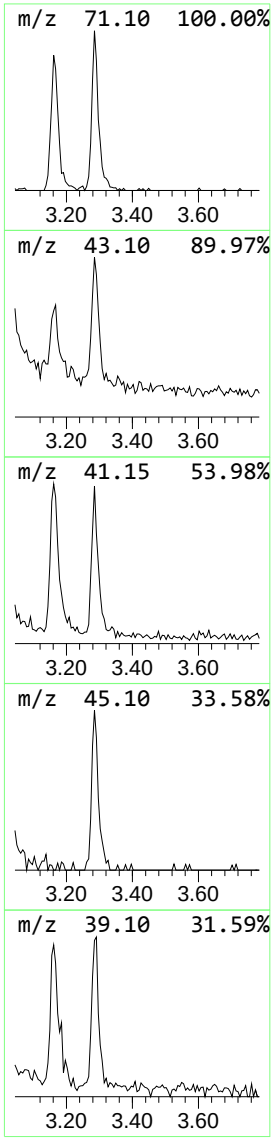
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1-Propene, 3-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.285	8.18 ng	97923	1,4-Dichlorobenzene-d4	8.115

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 3-methoxy-2-methyl-	86	C5H10O	022418-49-1	56
2	Pantolactone	130	C6H10O3	000599-04-2	45
3	3-Penten-2-ol	86	C5H10O	001569-50-2	45
4	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	45
5	Z-1-Methoxy-2-pentene	100	C6H12O	1000279-59-4	38





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Data File : BG048979.D
Acq On : 15 Jun 2021 15:57
Operator : CG/JU
Sample : M2672-19
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(80-84)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
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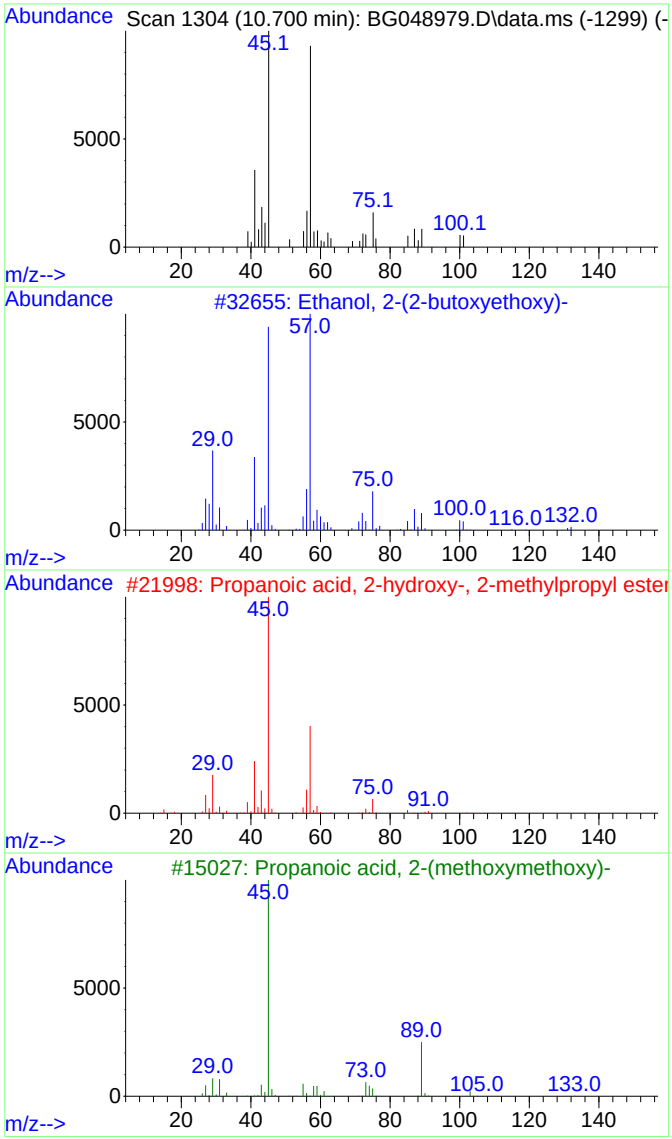
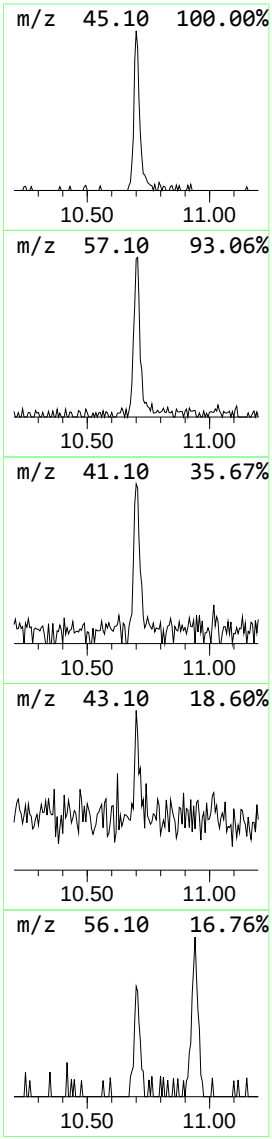
****

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.700	2.93 ng	47482	Naphthalene-d8	10.941

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	59
3	Propanoic acid, 2-(methoxymethoxy)-	134	C5H10O4	081327-29-9	47
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	40
5	1-Methoxy-3-methyl-3-butene	100	C6H12O	034752-58-4	38





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Data File : BG048979.D
Acq On : 15 Jun 2021 15:57
Operator : CG/JU
Sample : M2672-19
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(80-84)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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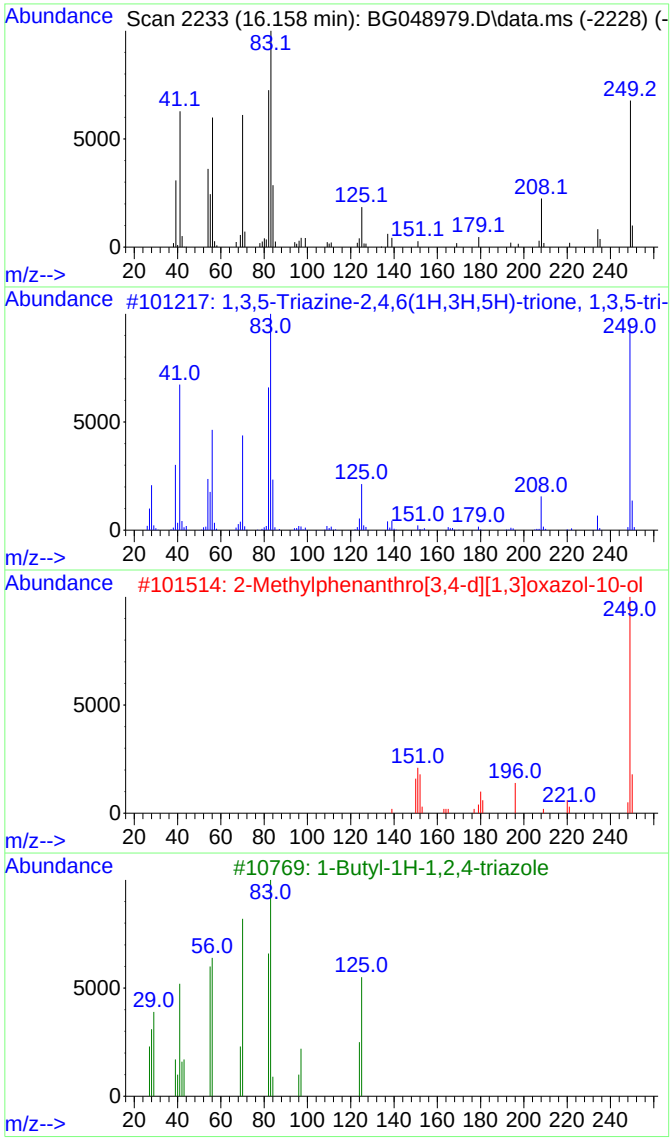
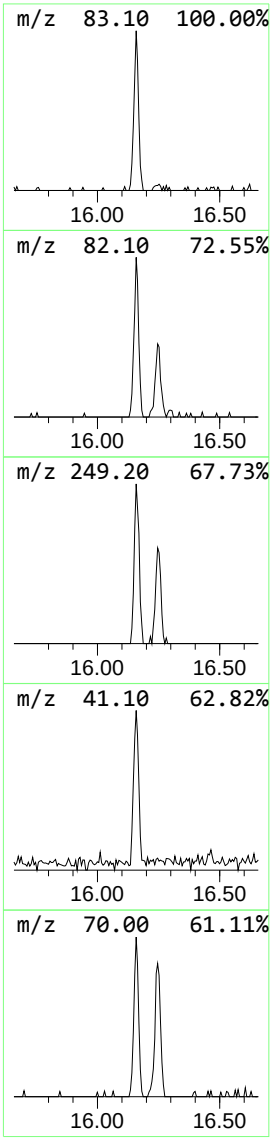
****

Peak Number 4 1,3,5-Triazine-2,4,6(1H,3H,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.158	3.24 ng	93634	Phenanthrene-d10	17.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Triazine-2,4,6(1H,3H,5H)-t...	249	C12H15N3O3	001025-15-6	97
2	2-Methylphenanthro[3,4-d][1,3]ox...	249	C16H11NO2	098033-24-0	47
3	1-Butyl-1H-1,2,4-triazole	125	C6H11N3	006086-22-2	37
4	Cyclohexane, undecyl-	238	C17H34	054105-66-7	17
5	Cyclohexane, eicosyl-	364	C26H52	004443-55-4	17





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Sample : M2672-19
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(80-84)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
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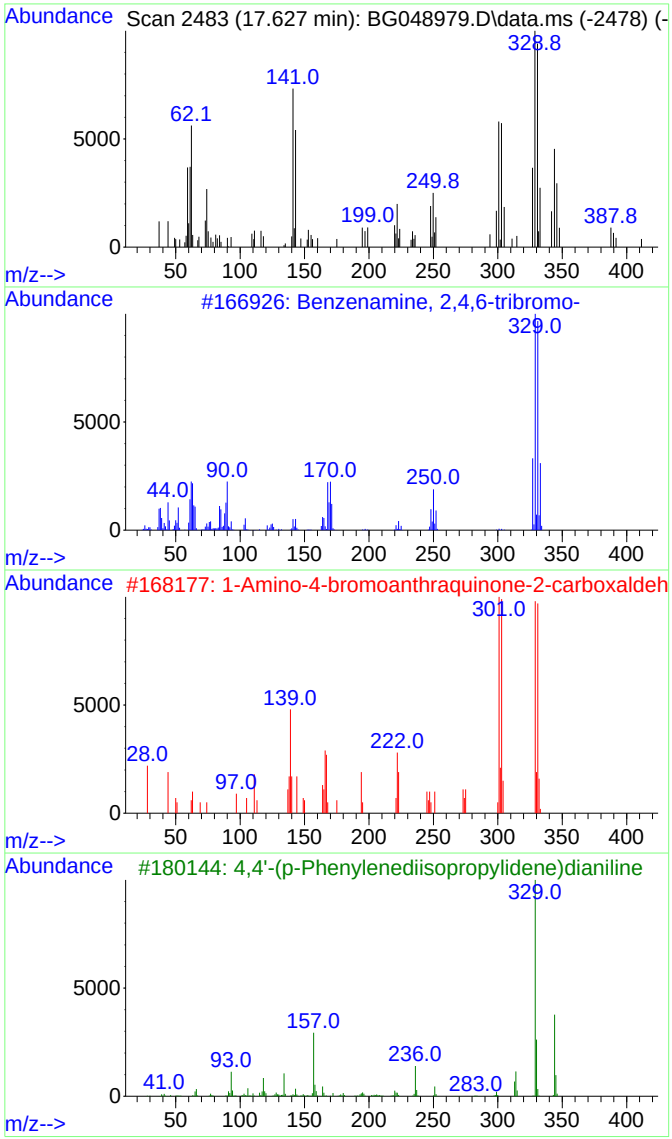
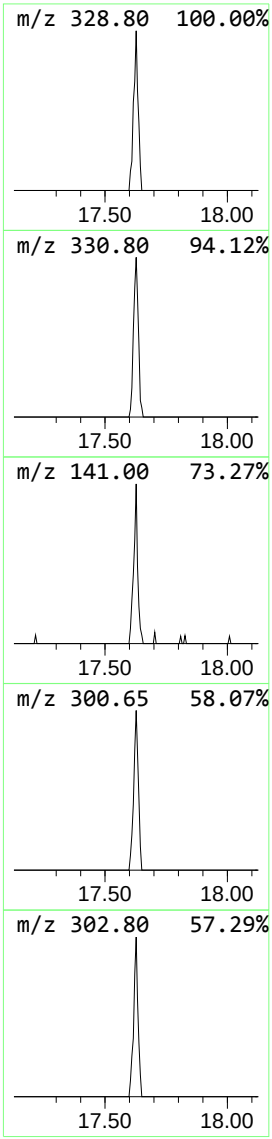
****

Peak Number 5 unknown17.627 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.627	2.56 ng	73993	Phenanthrene-d10	17.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenamine, 2,4,6-tribromo-	327	C6H4Br3N	000147-82-0	46
2	1-Amino-4-bromoanthraquinone-2-c...	329	C15H8BrNO3	062823-21-6	16
3	4,4'-(p-Phenylenediisopropyliden...	344	C24H28N2	002716-10-1	11
4	Bromophos	364	C8H8BrCl2O3PS	002104-96-3	10
5	2,5-Di(trifluoroacetyloxy)acetop...	344	C12H6F6O5	1000365-30-5	9





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Misc :
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Instrument :
BNA_G
ClientSampleId :
17-B6(80-84)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
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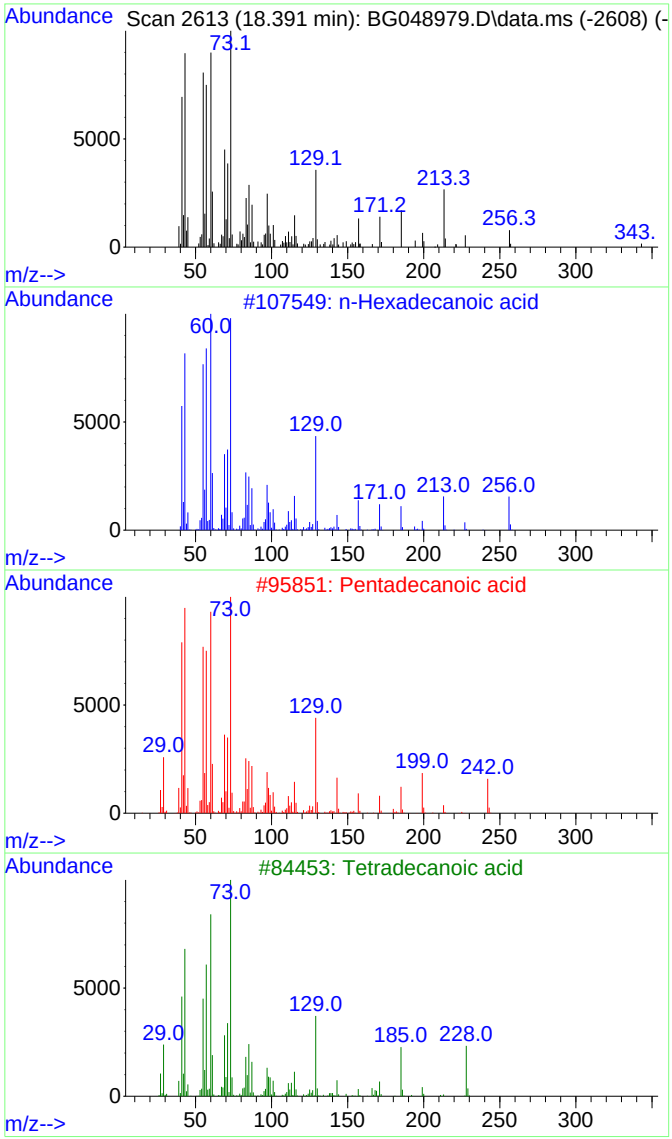
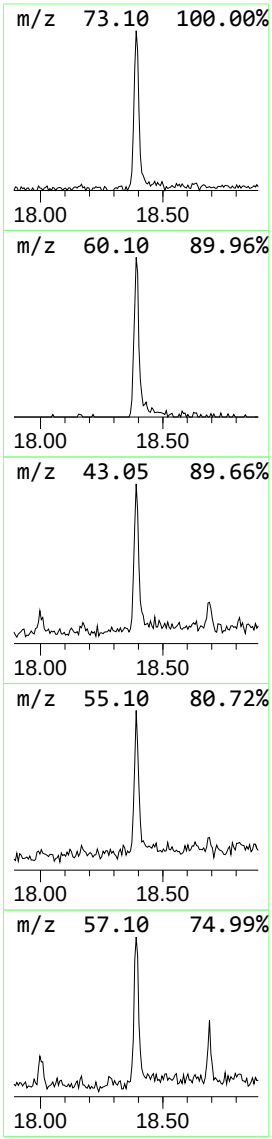
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.391	7.27 ng	210061	Phenanthrene-d10	17.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Dodecanoic acid	200	C12H24O2	000143-07-7	74
5	Tridecanoic acid	214	C13H26O2	000638-53-9	72





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Acq On : 15 Jun 2021 15:57
Operator : CG/JU
Sample : M2672-19
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(80-84)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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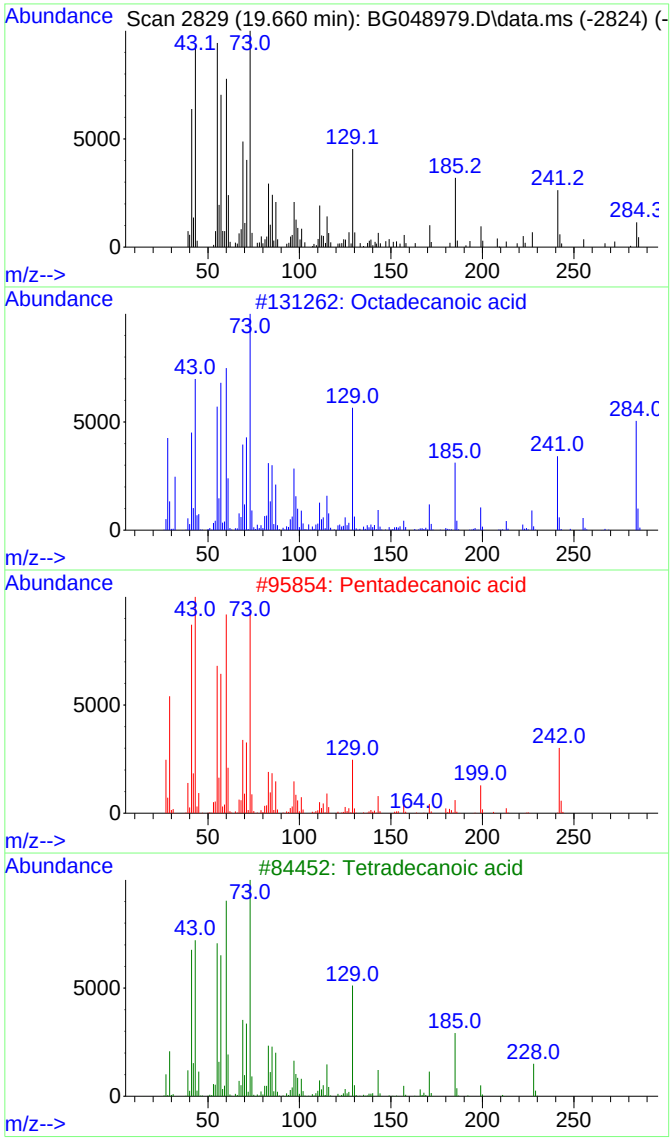
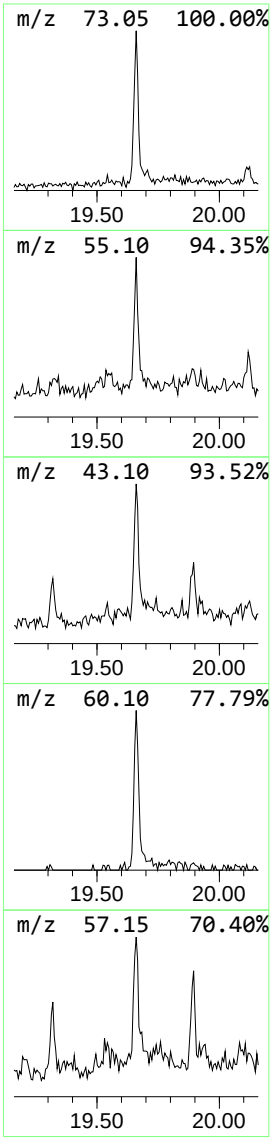
Peak Number 7 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.660	4.97 ng	163123	Chrysene-d12	21.799

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	76
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	59





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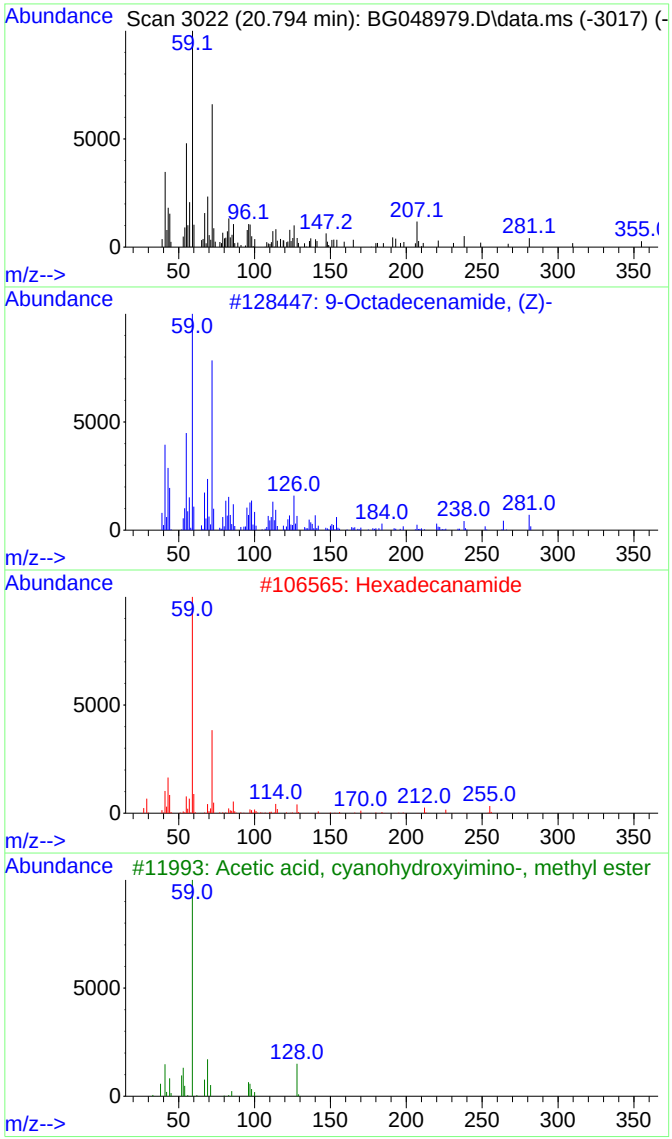
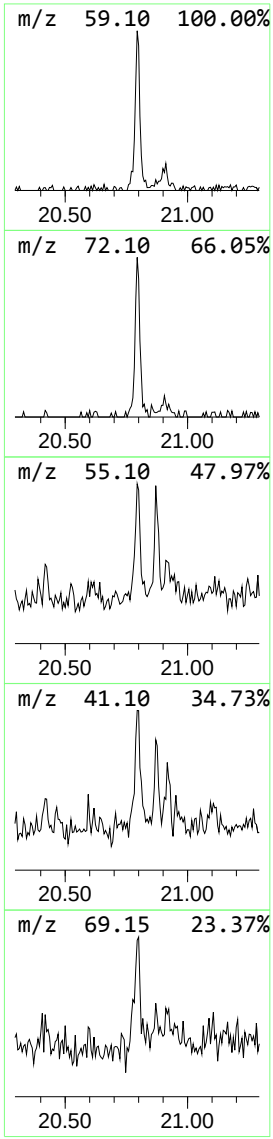
****

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.794	2.91 ng	95512	Chrysene-d12	21.799

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	83
2	Hexadecanamide	255	C16H33NO	000629-54-9	59
3	Acetic acid, cyanohydroxyimino-,...	128	C4H4N2O3	061295-92-9	43
4	2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	38
5	7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	35





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Data File : BG048979.D
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Operator : CG/JU
Sample : M2672-19
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(80-84)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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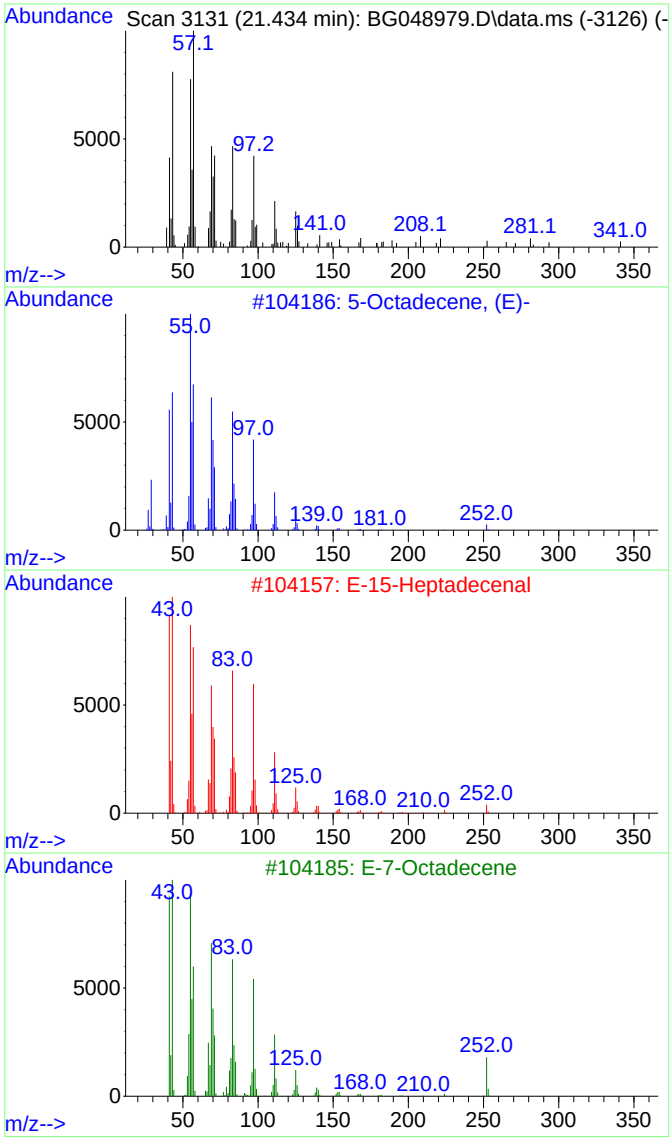
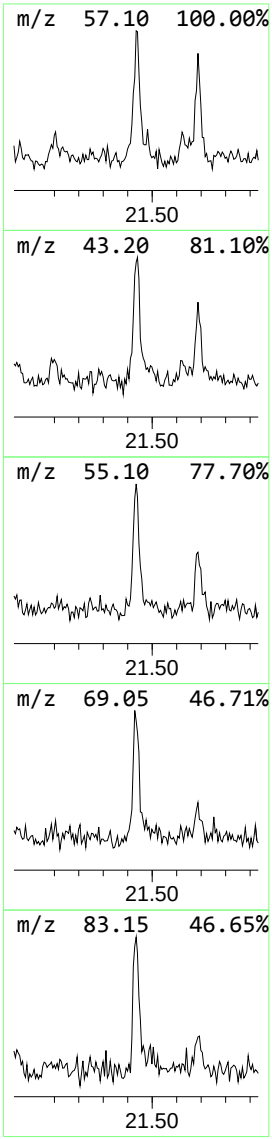
****

Peak Number 9 5-Octadecene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.434	3.49 ng	114492	Chrysene-d12	21.799

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	86
2	E-15-Heptadecenal	252	C17H32O	1000130-97-9	83
3	E-7-Octadecene	252	C18H36	1000130-92-0	83
4	17-Pentatriacontene	491	C35H70	006971-40-0	83
5	1-Octadecene	252	C18H36	000112-88-9	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048979.D
Acq On : 15 Jun 2021 15:57
Operator : CG/JU
Sample : M2672-19
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
17-B6(80-84)

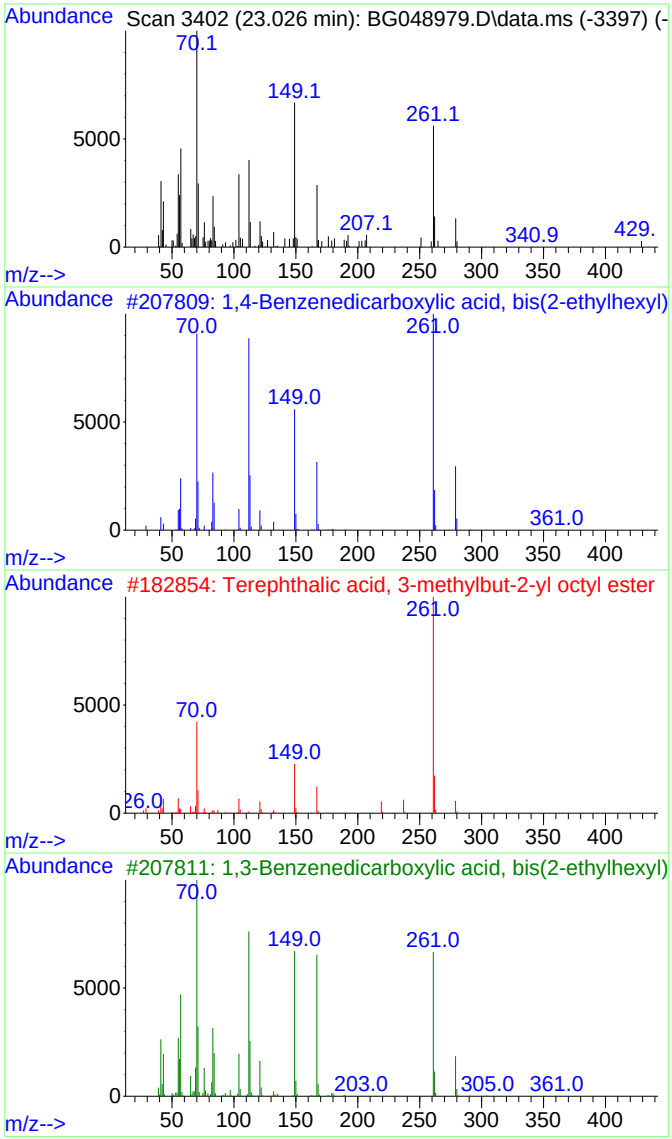
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

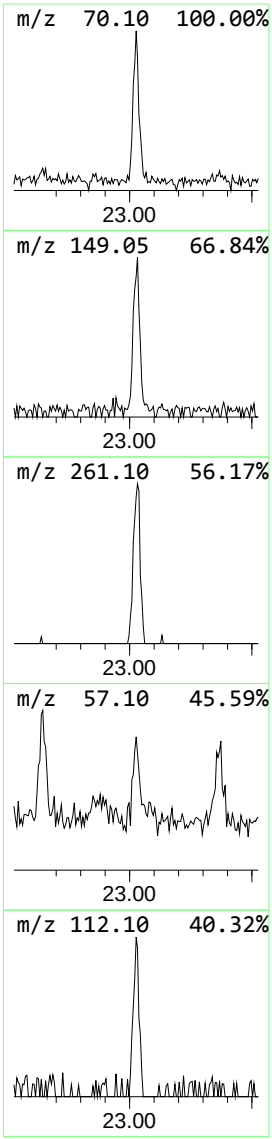
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1,4-Benzenedicarboxylic aci... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.026	2.58 ng	84740	Chrysene-d12	21.799

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	50
2	Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	47
3	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	47
4	2-Heptene, 3-methyl-	112	C8H16	003404-75-9	35
5	Isophthalic acid, di(4-octyl) ester	390	C24H38O4	1000344-04-3	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048979.D
Acq On : 15 Jun 2021 15:57
Operator : CG/JU
Sample : M2672-19
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(80-84)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-chlor...	3.162	11.9	ng	141824	1	8.115	239452	20.0
1-Propene, 3-me...	3.285	8.2	ng	97923	1	8.115	239452	20.0
Ethanol, 2-(2-b...	10.700	2.9	ng	47482	2	10.941	323627	20.0
1,3,5-Triazine-...	16.158	3.2	ng	93634	4	17.509	578119	20.0
unknown17.627	17.627	2.6	ng	73993	4	17.509	578119	20.0
n-Hexadecanoic ...	18.391	7.3	ng	210061	4	17.509	578119	20.0
Octadecanoic acid	19.660	5.0	ng	163123	5	21.799	656408	20.0
9-Octadecenamid...	20.794	2.9	ng	95512	5	21.799	656408	20.0
5-Octadecene, (E)-	21.434	3.5	ng	114492	5	21.799	656408	20.0
1,4-Benzenedica...	23.026	2.6	ng	84740	5	21.799	656408	20.0