LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061621\
Data File : BG048999.D
Acq On : 16 Jun 2021 14:54
Operator : CG/JU
Sample : M2672-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(16-20)

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: BG048999.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	16	21	30	rBV	137226	234749	8.15%	1.693%
2	3.285	38	42	53	rVB2	56993	85072	2.95%	0.614%
3	5.194	361	367	374	rBV	23219	38954	1.35%	0.281%
4	5.664	440	447	455	rBV	743613	1222520	42.44%	8.818%
5	5.735	455	459	468	rVB3	17271	42144	1.46%	0.304%
6	7.268	712	720	731	rBV	739230	1322743	45.91%	9.541%
7	8.115	857	864	869	rBV	129072	223443	7.76%	1.612%
8	9.278	1054	1062	1074	rVB	442670	824604	28.62%	5.948%
9	10.700	1298	1304	1312	rBV3	17551	34532	1.20%	0.249%
10	10.935	1336	1344	1352	rVB	163773	306767	10.65%	2.213%
11	13.379	1753	1760	1769	rBV	1114411	1729829	60.05%	12.477%
12	14.760	1988	1995	2005	rVB	278232	444589	15.43%	3.207%
13	16.158	2227	2233	2239	rVB2	39068	56056	1.95%	0.404%
14	16.246	2239	2248	2261	rBV	1007575	1605084	55.72%	11.577%
15	17.504	2454	2462	2469	rBV	357019	587911	20.41%	4.240%
16	17.621	2476	2482	2487	rVB4	44977	64720	2.25%	0.467%
17	18.162	2569	2574	2578	rBV2	38894	49690	1.72%	0.358%
18	18.385	2606	2612	2623	rBV2	70794	115499	4.01%	0.833%
19	19.536	2804	2808	2818	rVB3	46981	78137	2.71%	0.564%
20	19.654	2824	2828	2837	rBV2	59820	82849	2.88%	0.598%
21	19.795	2848	2852	2858	rVB3	22064	38597	1.34%	0.278%
22	20.112	2900	2906	2913	rBV	2129518	2880865	100.00%	20.779%
23	20.794	3014	3022	3030	rBV2	193297	301591	10.47%	2.175%
24	20.900	3037	3040	3046	rVB4	24094	42992	1.49%	0.310%
25	21.428	3126	3130	3138	rVB4	58700	94753	3.29%	0.683%
26	21.681	3169	3173	3181	rVB	42499	63058	2.19%	0.455%
27	21.799	3186	3193	3199	rBV	351160	618814	21.48%	4.463%
28	23.021	3396	3401	3411	rVB	25652	54424	1.89%	0.393%
29	25.124	3750	3759	3770	rBV2	206752	619210	21.49%	4.466%

Sum of corrected areas: 13864196

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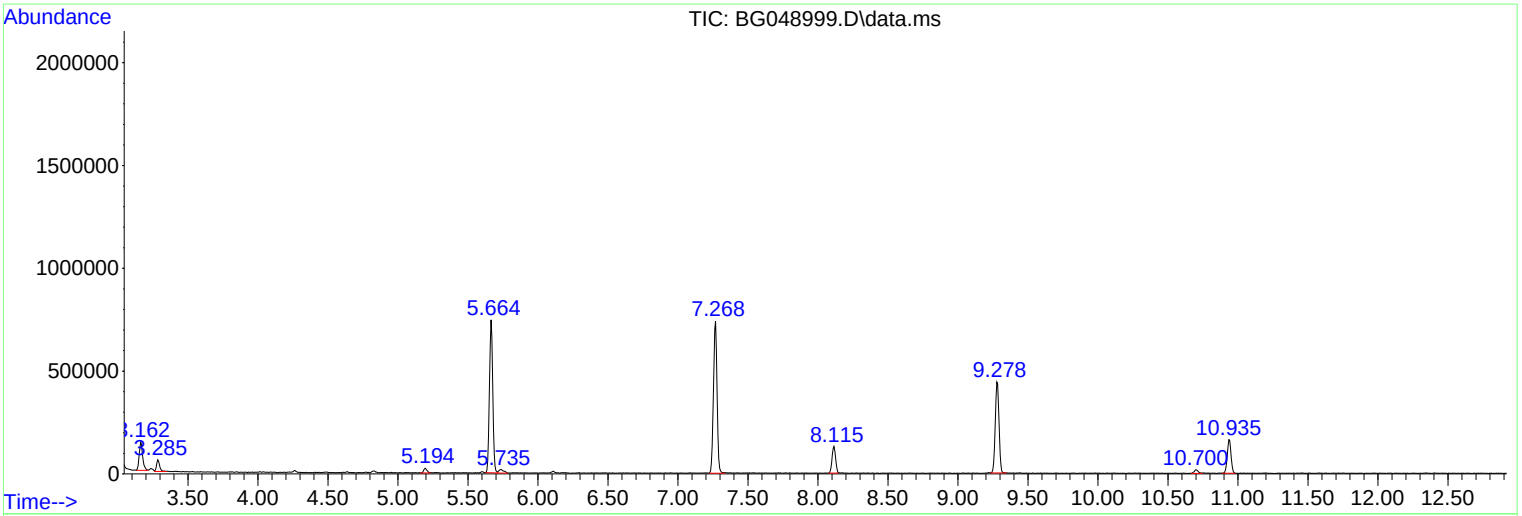
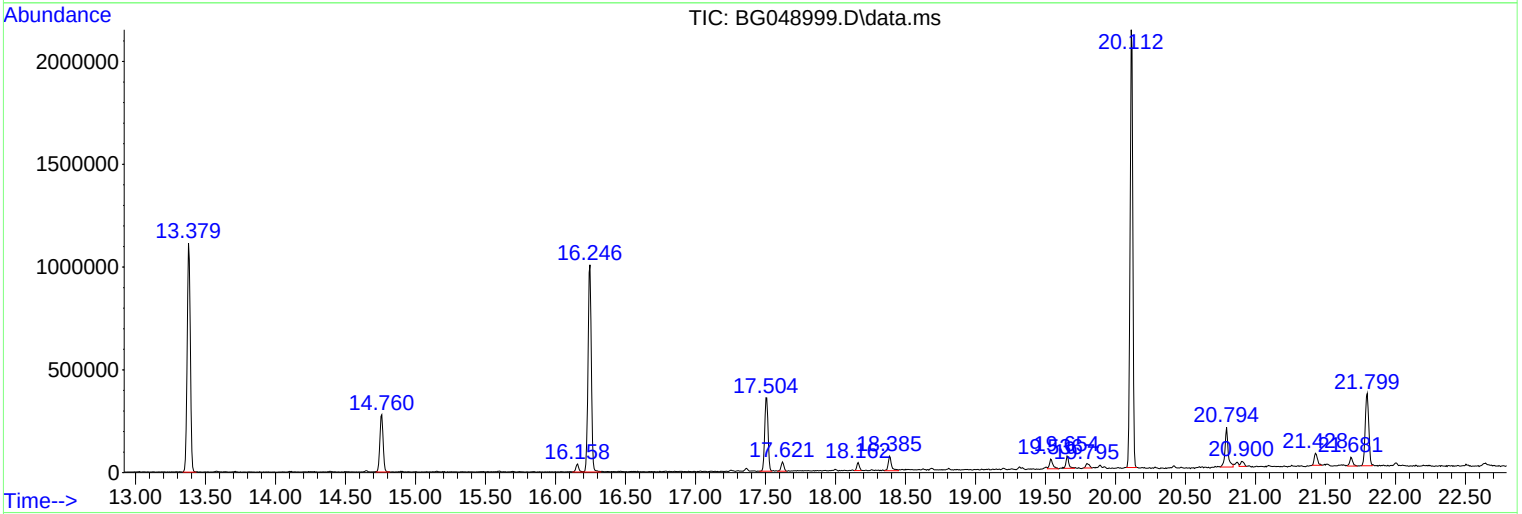
Misc :
ALS Vial : 9 Sample Multiplier: 1

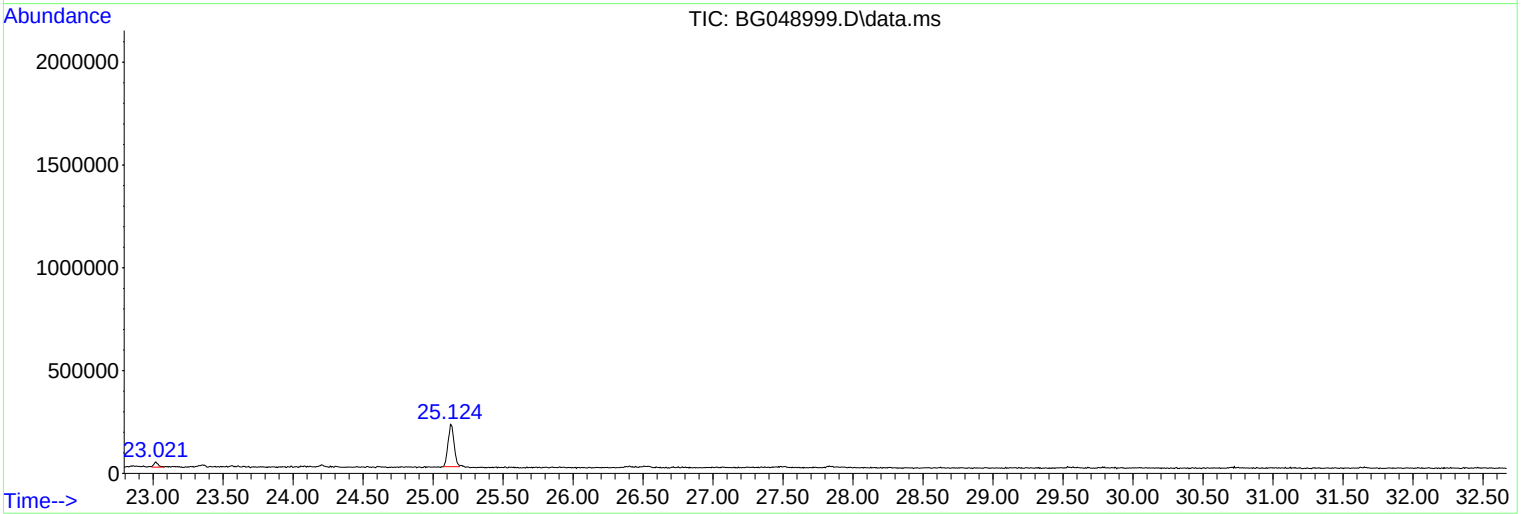
Instrument :
BNA_G
ClientSampleId :
17-B6(16-20)

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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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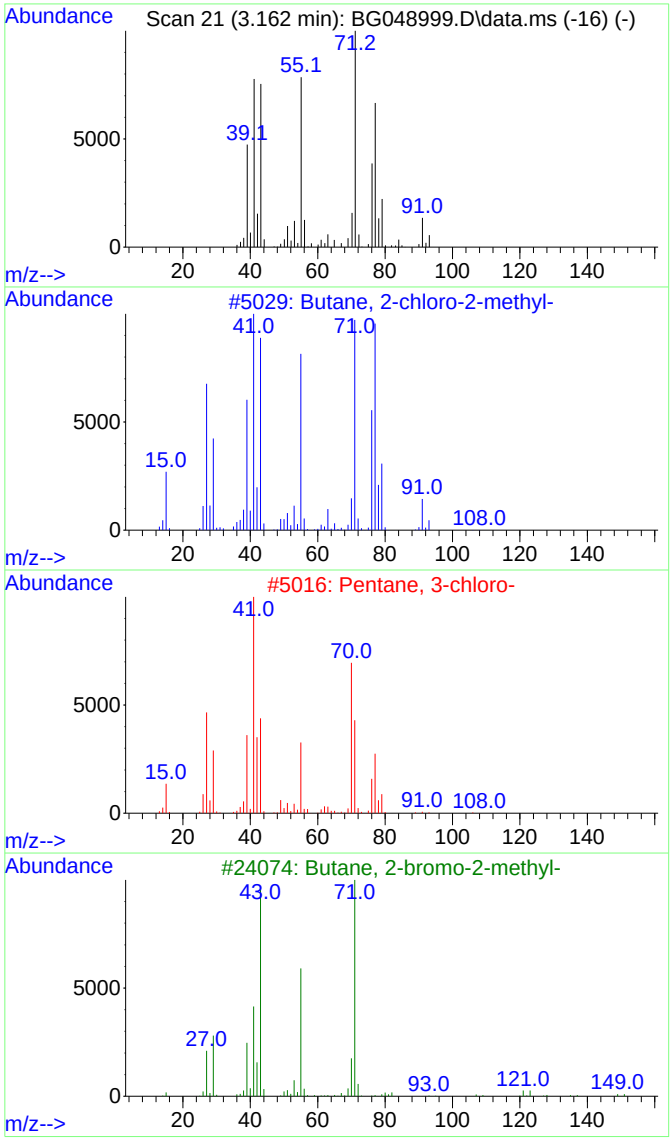
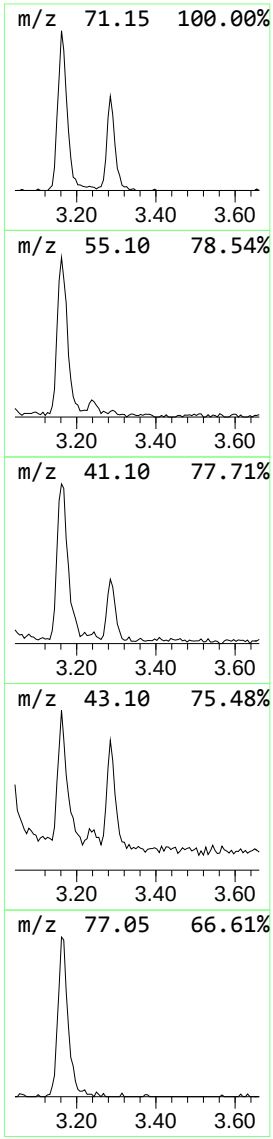
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.162	21.01 ng	234749	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	83
2	Pentane, 3-chloro-	106	C5H11Cl	000616-20-6	36
3	Butane, 2-bromo-2-methyl-	150	C5H11Br	000507-36-8	22
4	Butyric acid, m-nitrophenyl ester	209	C10H11NO4	014617-97-1	22
5	1-Hexene, 4,5-dimethyl-	112	C8H16	016106-59-5	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061621\
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Operator : CG/JU
Sample : M2672-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
17-B6(16-20)

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

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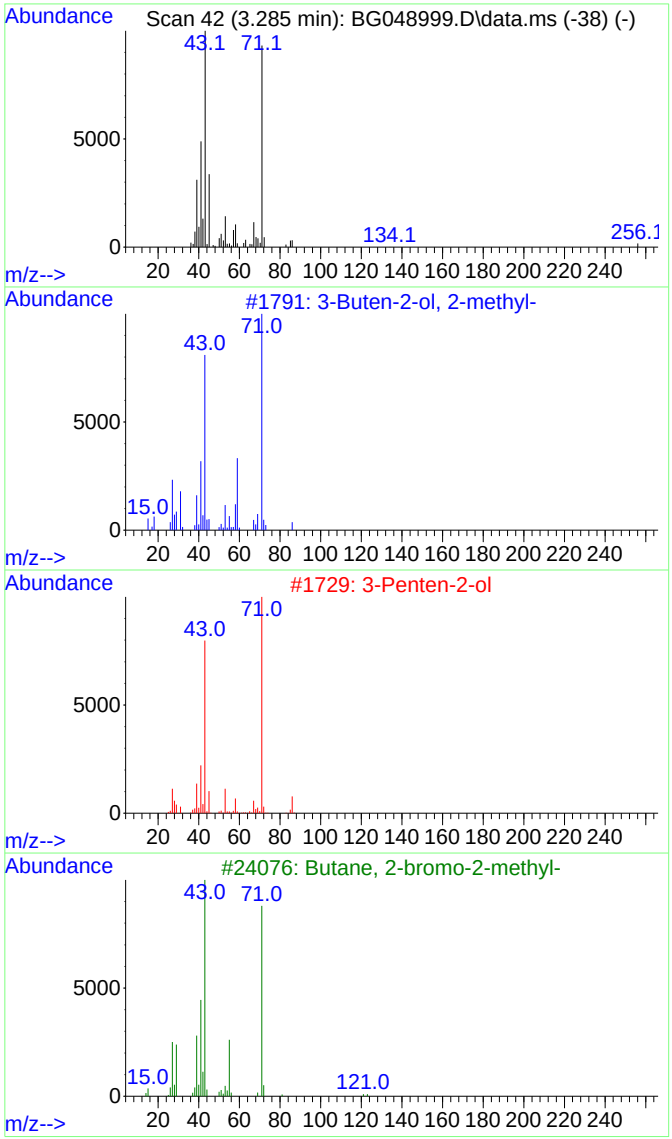
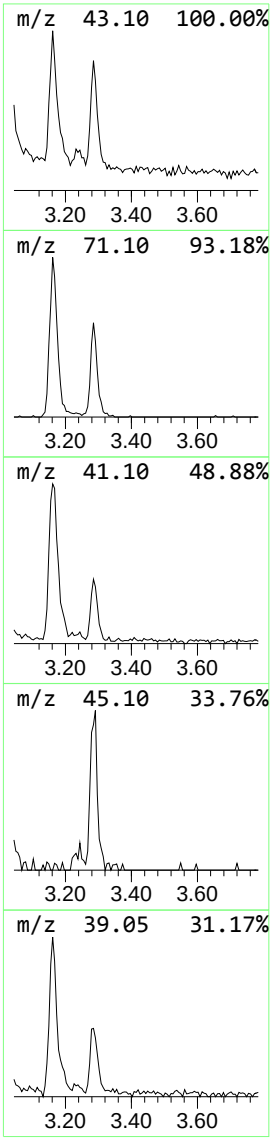
****
Peak Number 2 3-Buten-2-ol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.285	7.61 ng	85072	1,4-Dichlorobenzene-d4	8.115

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	64
2	3-Penten-2-ol	86	C5H10O	001569-50-2	56
3	Butane, 2-bromo-2-methyl-	150	C5H11Br	000507-36-8	53
4	Acetic acid, (1,2-dimethyl-1-pro...	128	C7H12O2	003814-41-3	50
5	Z-1-Methoxy-2-pentene	100	C6H12O	1000279-59-4	50





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Data File : BG048999.D
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Operator : CG/JU
Sample : M2672-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(16-20)

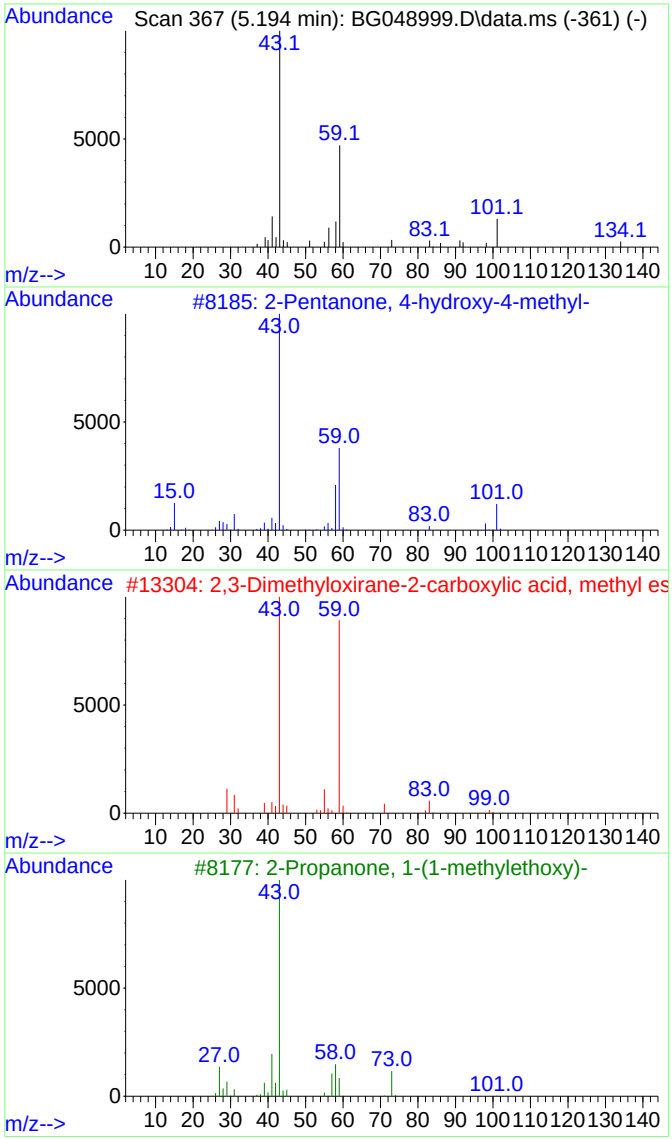
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

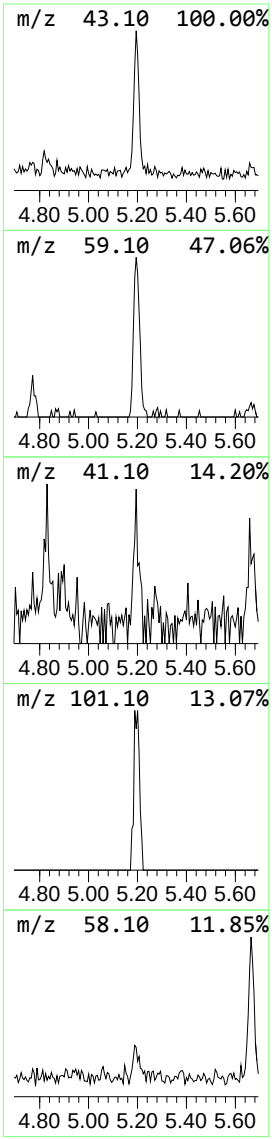
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.194	3.49 ng	38954	1,4-Dichlorobenzene-d4	8.115

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2	2,3-Dimethyloxirane-2-carboxylic...	130	C6H10O3	1000306-64-4	25
3	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	10
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Diacetamide	101	C4H7NO2	000625-77-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061621\
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Acq On : 16 Jun 2021 14:54
Operator : CG/JU
Sample : M2672-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(16-20)

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

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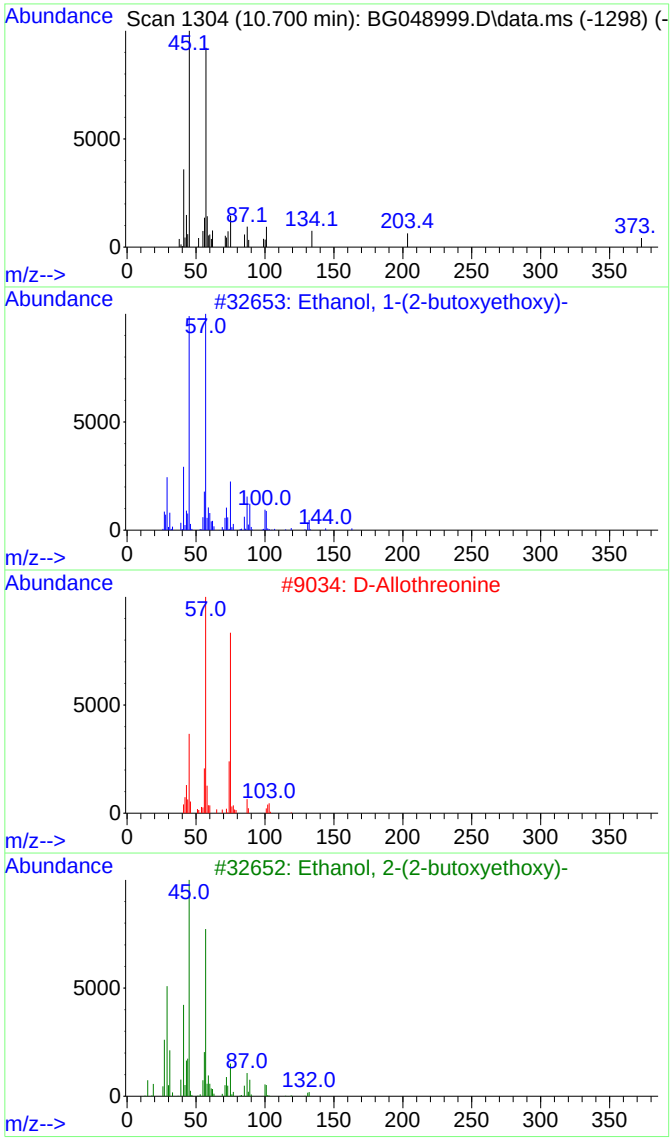
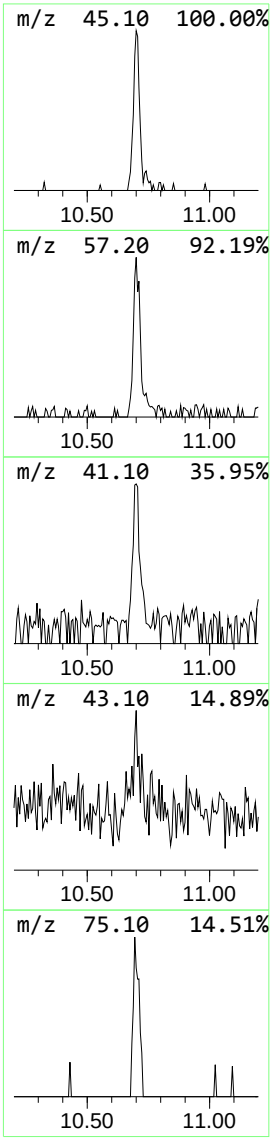
****

Peak Number 5 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.700	2.25 ng	34532	Naphthalene-d8	10.935

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50
2	D-Allothreonine	119	C4H9NO3	024830-94-2	45
3	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	45
4	2-Propanol, 1-(2-methylpropoxy)-	132	C7H16O2	023436-19-3	42
5	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	40





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Operator : CG/JU
Sample : M2672-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
17-B6(16-20)

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

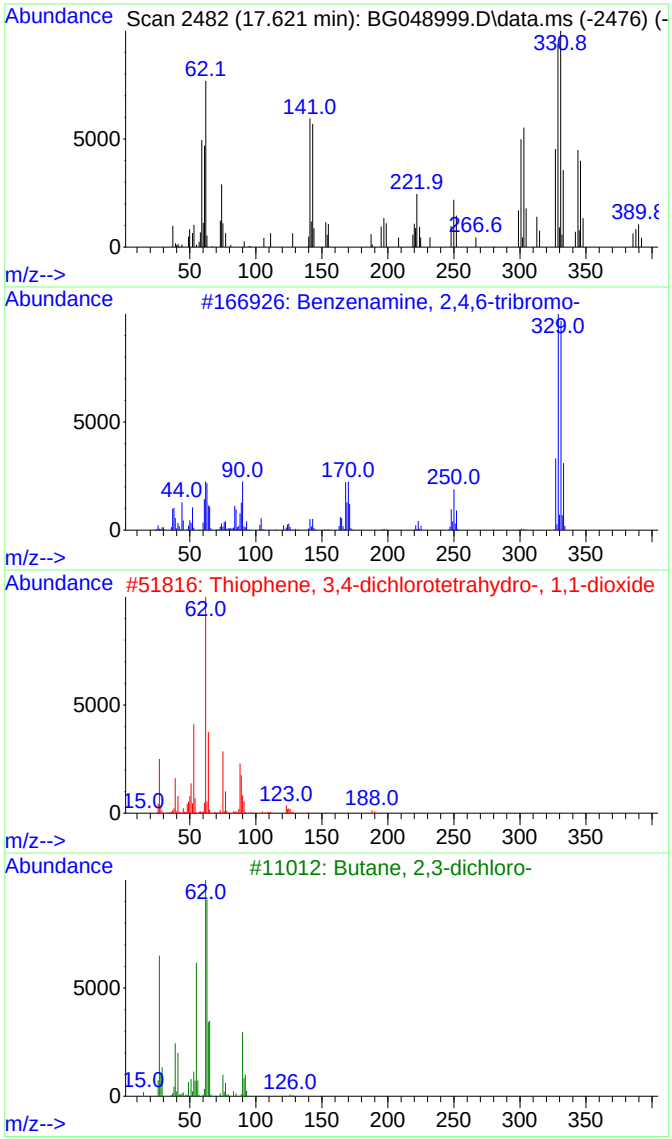
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

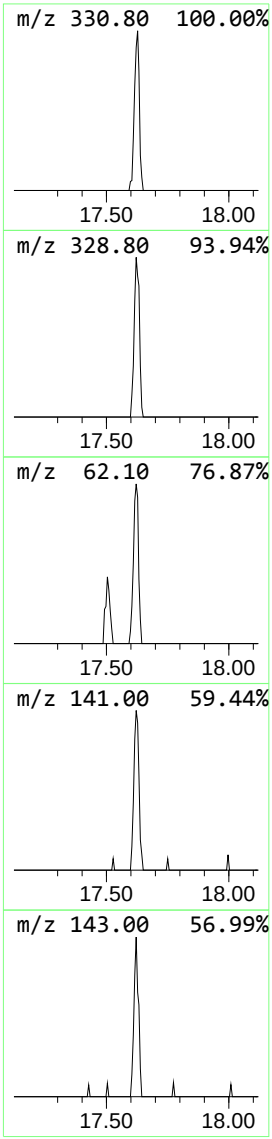
****

Peak Number 6 Benzenamine, 2,4,6-tribromo- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.621	2.20 ng	64720	Phenanthrene-d10	17.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenamine, 2,4,6-tribromo-	327	C6H4Br3N	000147-82-0	70
2	Thiophene, 3,4-dichlorotetrahydr...	188	C4H6Cl2O2S	003001-57-8	17
3	Butane, 2,3-dichloro-	126	C4H8Cl2	007581-97-7	17
4	Triethylphosphine	118	C6H15P	000554-70-1	17
5	1H-Pyrazolo[4,3-c]pyridazin-3-ol...	388	C22H20N4O3	035426-81-4	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061621\
Data File : BG048999.D
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Operator : CG/JU
Sample : M2672-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(16-20)

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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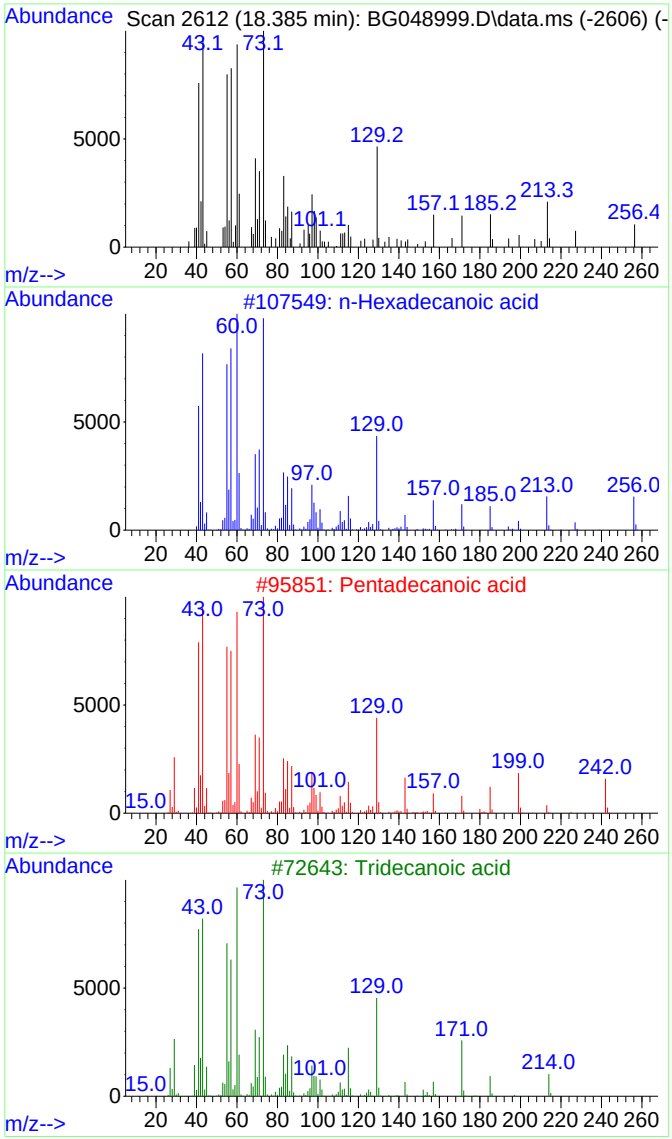
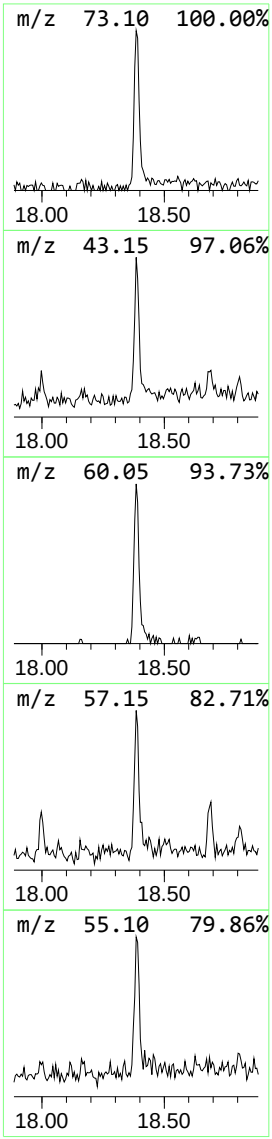
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.385	3.93 ng	115499	Phenanthrene-d10	17.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
3	Tridecanoic acid	214	C13H26O2	000638-53-9	62
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5	n-Decanoic acid	172	C10H20O2	000334-48-5	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061621\
Data File : BG048999.D
Acq On : 16 Jun 2021 14:54
Operator : CG/JU
Sample : M2672-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(16-20)

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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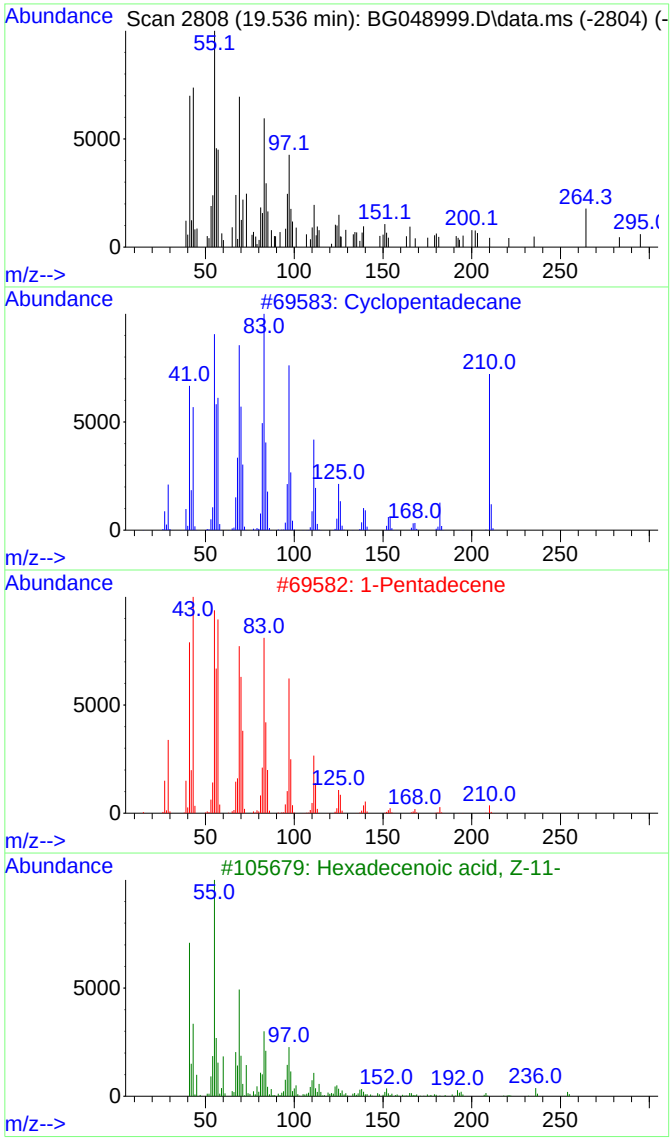
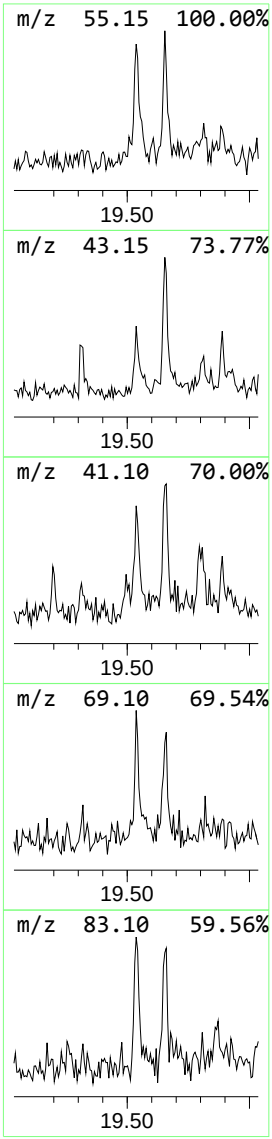
****

Peak Number 8 Cyclopentadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.536	2.66 ng	78137	Phenanthrene-d10	17.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	89
2	1-Pentadecene	210	C15H30	013360-61-7	89
3	Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	86
4	n-Pentadecanol	228	C15H32O	000629-76-5	68
5	Oleic Acid	282	C18H34O2	000112-80-1	64





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Operator : CG/JU
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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(16-20)

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TIC Library : C:\Database\NIST11.L
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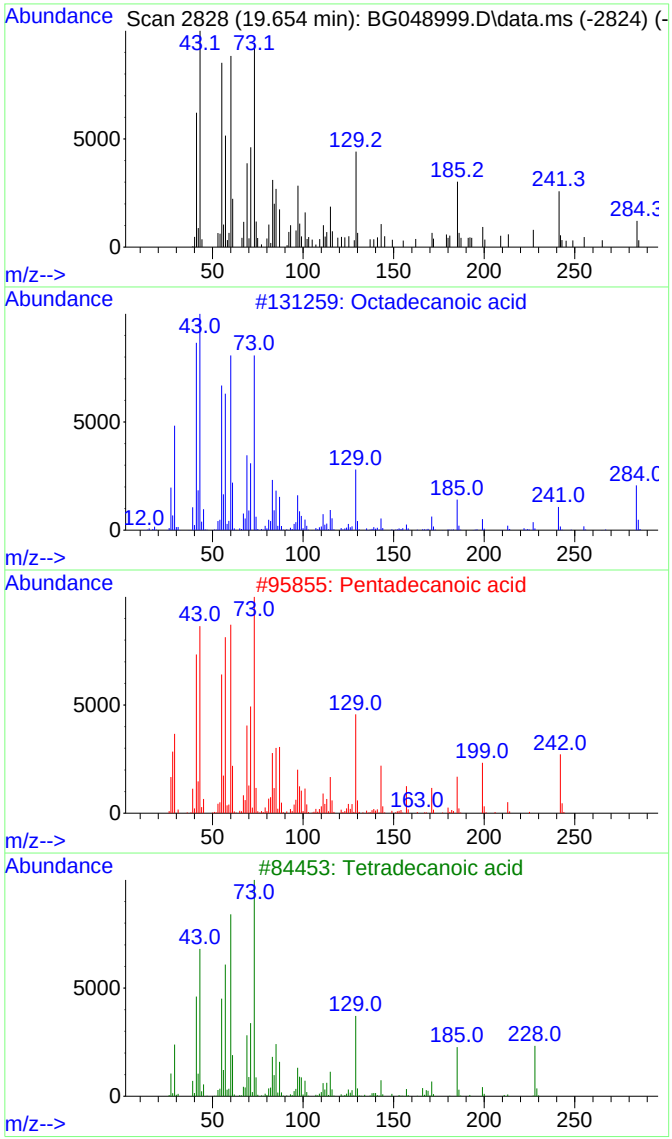
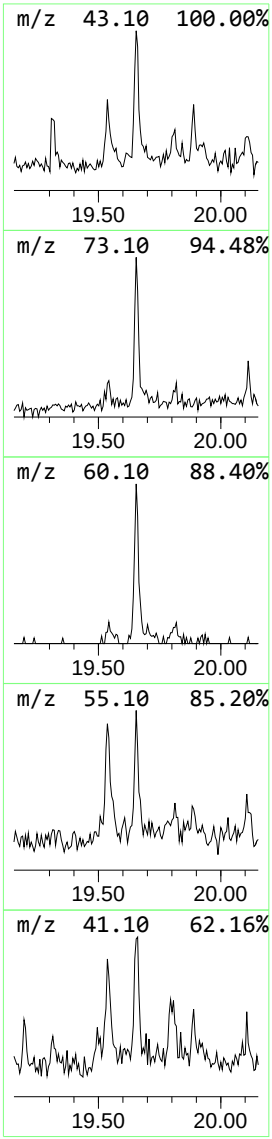
Peak Number 9 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.654	2.68 ng	82849	Chrysene-d12	21.799

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	n-Decanoic acid	172	C10H20O2	000334-48-5	58
5	Dodecanoic acid	200	C12H24O2	000143-07-7	52





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Data File : BG048999.D
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Operator : CG/JU
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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(16-20)

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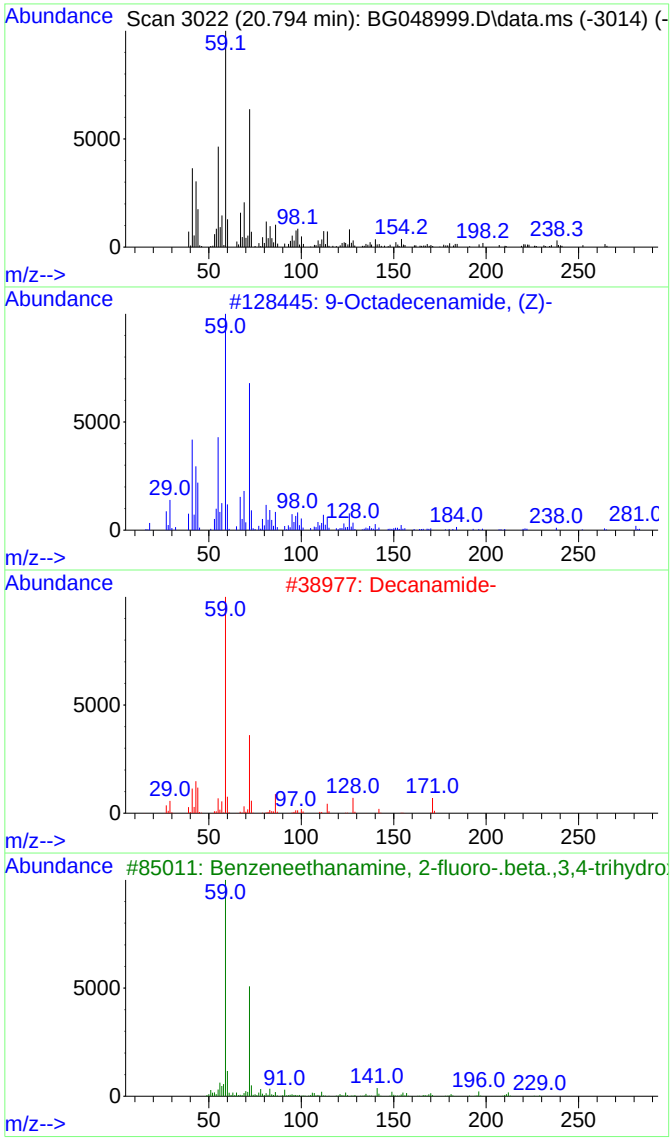
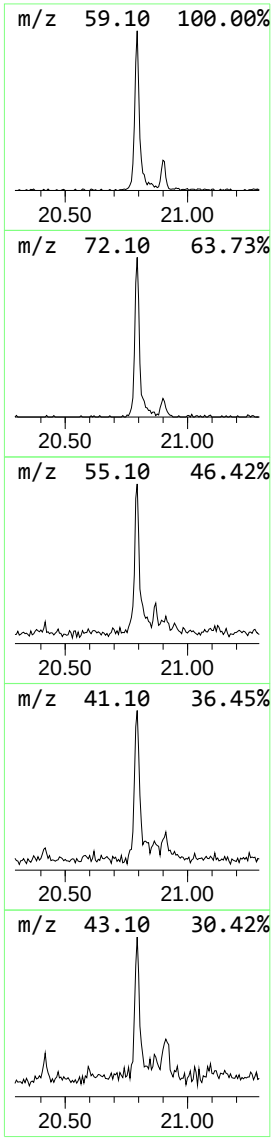
****

Peak Number 10 9-Octadecenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.794	9.75 ng	301591	Chrysene-d12	21.799

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
2	Decanamide-	171	C10H21NO	002319-29-1	64
3	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	64
4	Tetradecanamide	227	C14H29NO	000638-58-4	64
5	Octanamide	143	C8H17NO	000629-01-6	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061621\
Data File : BG048999.D
Acq On : 16 Jun 2021 14:54
Operator : CG/JU
Sample : M2672-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(16-20)

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

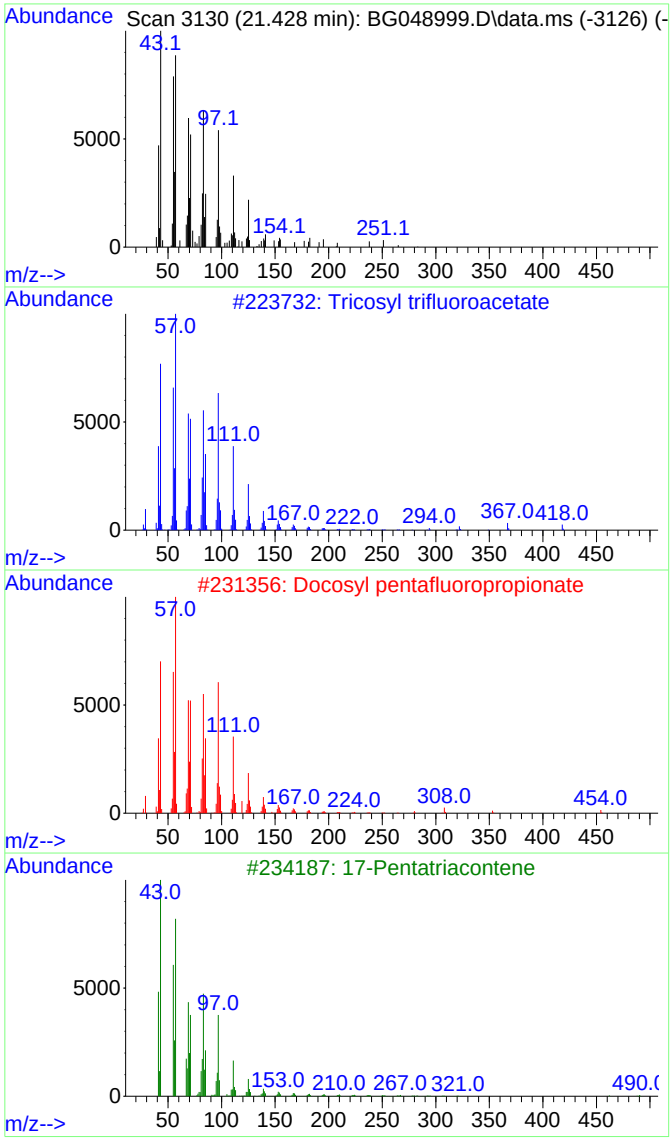
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

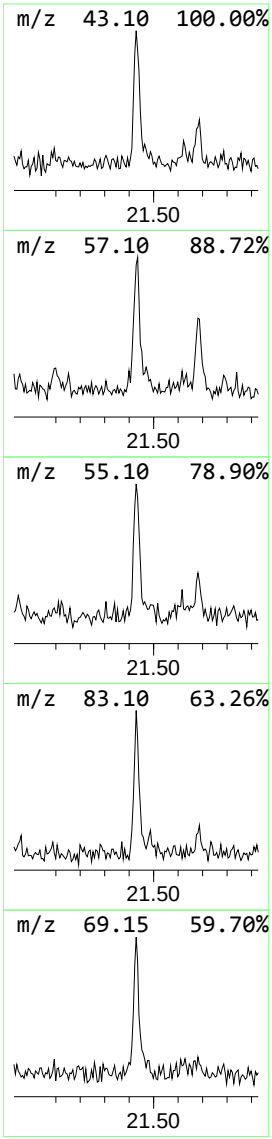
****

Peak Number 11 Tricosyl trifluoroacetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.428	3.06 ng	94753	Chrysene-d12	21.799

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
2	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	90
3	17-Pentatriacontene	491	C35H70	006971-40-0	87
4	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	80
5	Cyclooctadecane, ethyl-	280	C20H40	1000151-22-5	74





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061621\
Data File : BG048999.D
Acq On : 16 Jun 2021 14:54
Operator : CG/JU
Sample : M2672-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(16-20)

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	21.0	ng	234749	1	8.115	223443	20.0
3-Buten-2-ol, 2...	3.285	7.6	ng	85072	1	8.115	223443	20.0
2-Pentanone, 4-...	5.194	3.5	ng	38954	1	8.115	223443	20.0
Ethanol, 1-(2-b...	10.700	2.3	ng	34532	2	10.935	306767	20.0
Benzenamine, 2,...	17.621	2.2	ng	64720	4	17.509	587911	20.0
n-Hexadecanoic ...	18.385	3.9	ng	115499	4	17.509	587911	20.0
Cyclopentadecane	19.536	2.7	ng	78137	4	17.509	587911	20.0
Octadecanoic acid	19.654	2.7	ng	82849	5	21.799	618814	20.0
9-Octadecenamid...	20.794	9.8	ng	301591	5	21.799	618814	20.0
Tricosyl triflu...	21.428	3.1	ng	94753	5	21.799	618814	20.0