LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048978.D
Acq On : 15 Jun 2021 15:16
Operator : CG/JU
Sample : M2672-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(28-32)

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: BG048978.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.161	15	21	29	rBV2	139254	239256	8.84%	1.691%
2	3.285	38	42	52	rVB	61983	92631	3.42%	0.655%
3	5.194	362	367	373	rVB3	19527	35705	1.32%	0.252%
4	5.670	440	448	456	rBV	789330	1329236	49.12%	9.393%
5	5.735	456	459	468	rVB3	18229	40293	1.49%	0.285%
6	7.268	710	720	731	rBV	786353	1417590	52.38%	10.018%
7	8.114	858	864	871	rBV	137419	234469	8.66%	1.657%
8	9.283	1055	1063	1073	rVB	478490	882907	32.62%	6.239%
9	10.699	1299	1304	1313	rVB2	27088	47370	1.75%	0.335%
10	10.940	1336	1345	1353	rBV	176969	325096	12.01%	2.297%
11	13.385	1753	1761	1770	rVB	1076944	1693401	62.57%	11.967%
12	14.759	1985	1995	2003	rBV	275832	448601	16.58%	3.170%
13	16.158	2227	2233	2241	rBV2	37176	53589	1.98%	0.379%
14	16.246	2241	2248	2258	rBV	1084091	1639163	60.57%	11.584%
15	17.509	2456	2463	2469	rBV	366195	588886	21.76%	4.162%
16	17.627	2478	2483	2489	rBV5	41146	56540	2.09%	0.400%
17	18.167	2571	2575	2580	rVB3	23868	37729	1.39%	0.267%
18	18.390	2609	2613	2618	rBV	115744	158878	5.87%	1.123%
19	19.548	2806	2810	2818	rVB5	29015	58473	2.16%	0.413%
20	19.660	2825	2829	2834	rBV	92939	113261	4.19%	0.800%
21	19.801	2848	2853	2859	rBV2	48333	74478	2.75%	0.526%
22	20.118	2901	2907	2914	rVB	2057461	2706276	100.00%	19.125%
23	20.794	3016	3022	3027	rBV	84190	128418	4.75%	0.907%
24	20.923	3040	3044	3047	rVB4	23204	30635	1.13%	0.216%
25	21.434	3126	3131	3138	rBV2	84570	160421	5.93%	1.134%
26	21.687	3171	3174	3181	rVB2	45284	66298	2.45%	0.469%
27	21.798	3187	3193	3202	rBV2	370530	672789	24.86%	4.754%
28	22.004	3224	3228	3234	rVB5	26651	45877	1.70%	0.324%
29	22.644	3333	3337	3344	rVB4	26093	42499	1.57%	0.300%
30	23.026	3398	3402	3409	rVB7	34470	60980	2.25%	0.431%
31	25.135	3752	3761	3772	rBV2	224649	669026	24.72%	4.728%

Sum of corrected areas: 14150771

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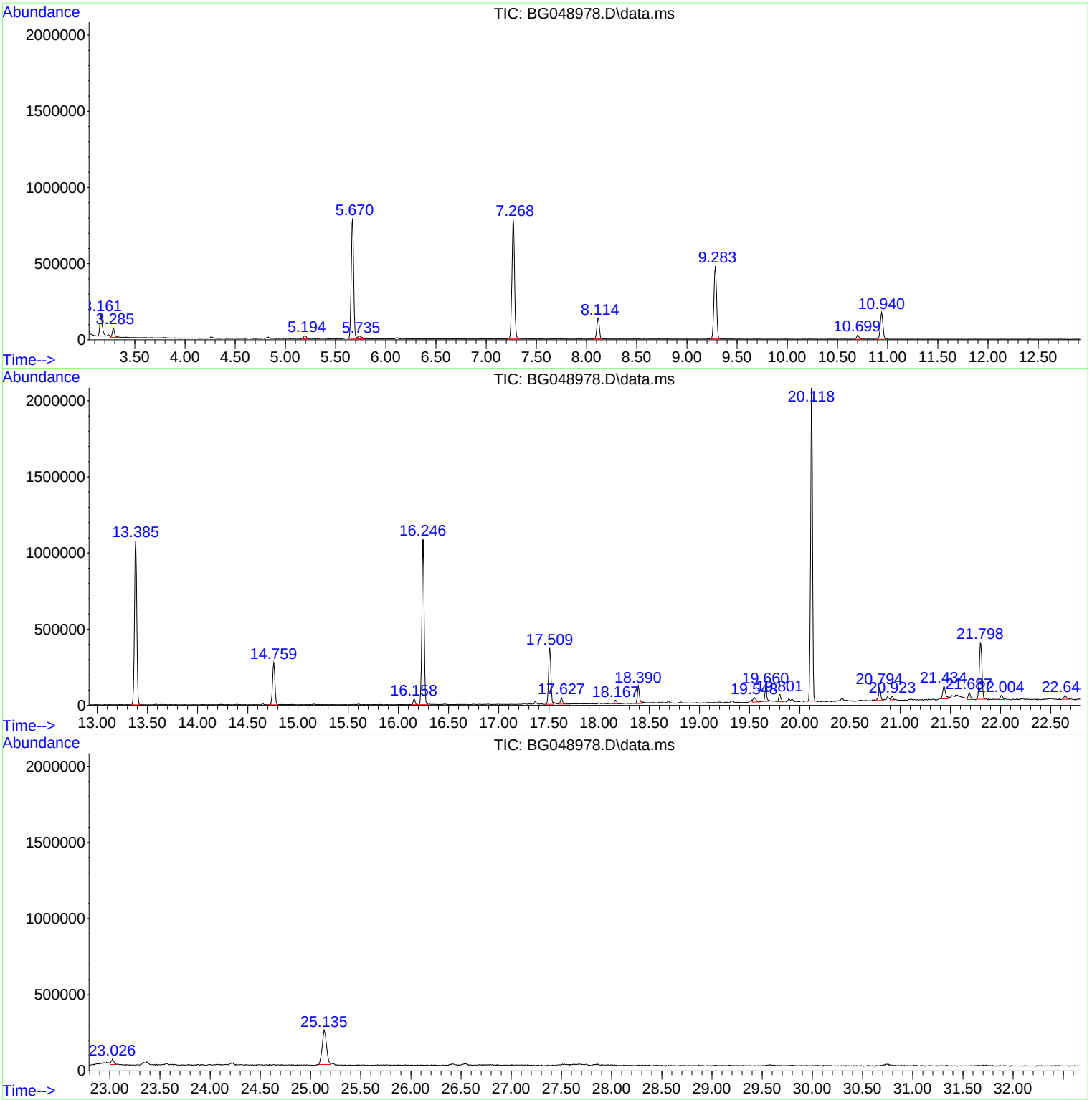
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
17-B6(28-32)

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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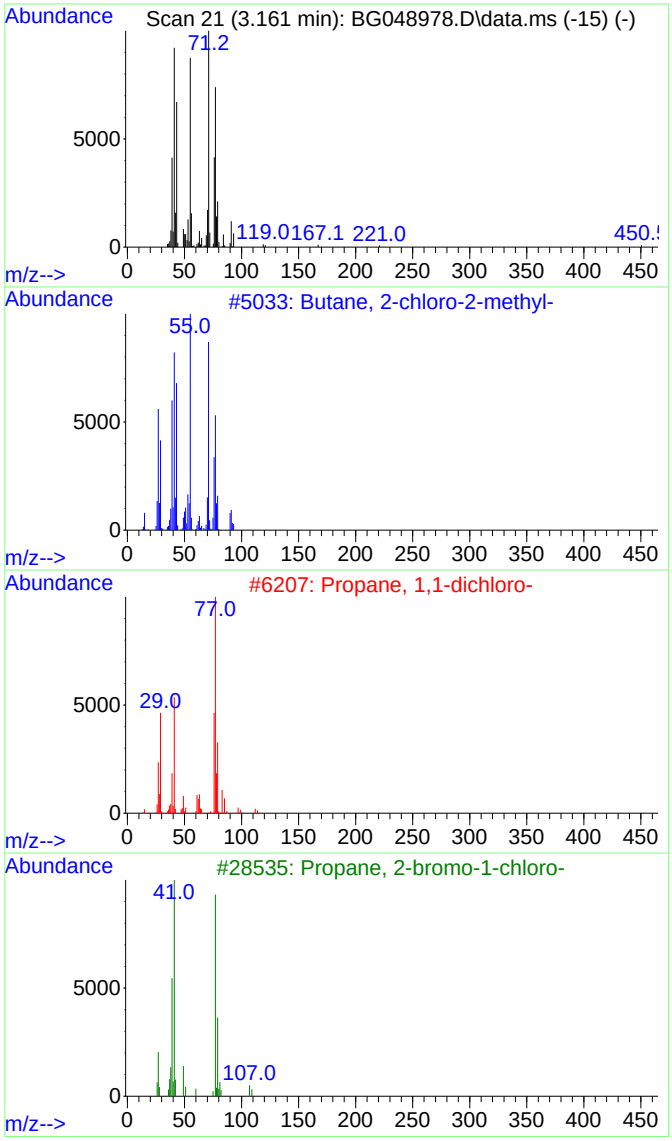
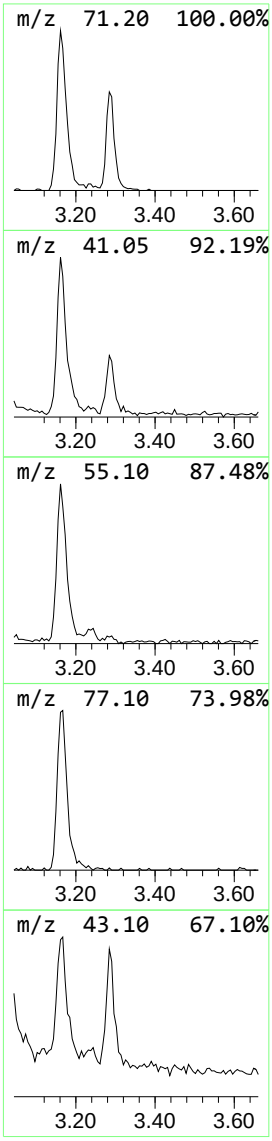
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.161	20.41 ng	239256	1,4-Dichlorobenzene-d4	8.120

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-chloro-2-methyl-	106	C5H11Cl	000594-36-5	83
2	Propane, 1,1-dichloro-	112	C3H6Cl2	000078-99-9	35
3	Propane, 2-bromo-1-chloro-	156	C3H6BrCl	003017-95-6	25
4	Butanoyl chloride, 2-chloro-	140	C4H6Cl2O	007623-11-2	22
5	1-Hexene, 4,5-dimethyl-	112	C8H16	016106-59-5	16





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Data File : BG048978.D
Acq On : 15 Jun 2021 15:16
Operator : CG/JU
Sample : M2672-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
17-B6(28-32)

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

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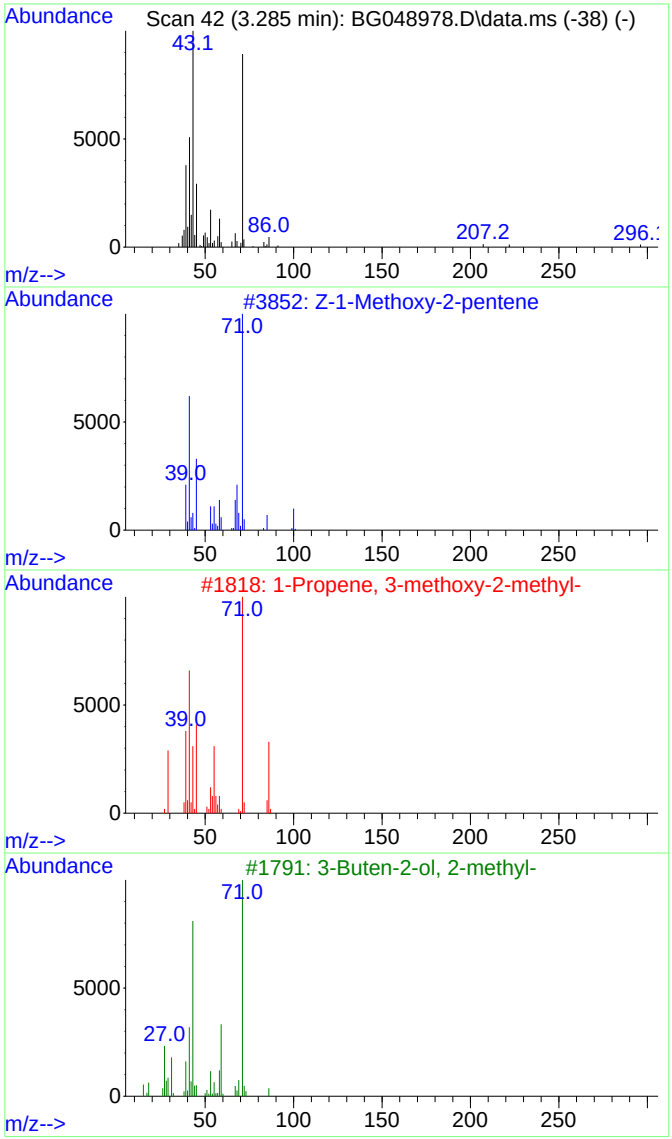
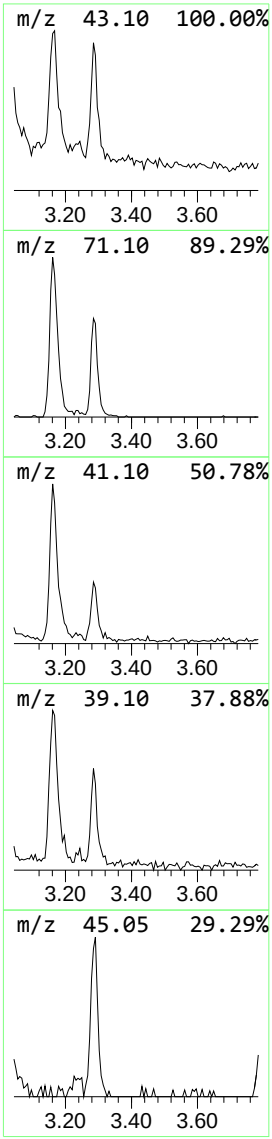
****

Peak Number 2 Z-1-Methoxy-2-pentene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.285	7.90 ng	92631	1,4-Dichlorobenzene-d4	8.120

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Z-1-Methoxy-2-pentene	100	C6H12O	1000279-59-4	78
2	1-Propene, 3-methoxy-2-methyl-	86	C5H10O	022418-49-1	72
3	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	64
4	2-Butene, 1-methoxy-, (E)-	86	C5H10O	010034-14-7	56
5	3-Chloro-2-buten-1-ol	106	C4H7ClO	040605-42-3	53





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Data File : BG048978.D
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Operator : CG/JU
Sample : M2672-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(28-32)

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

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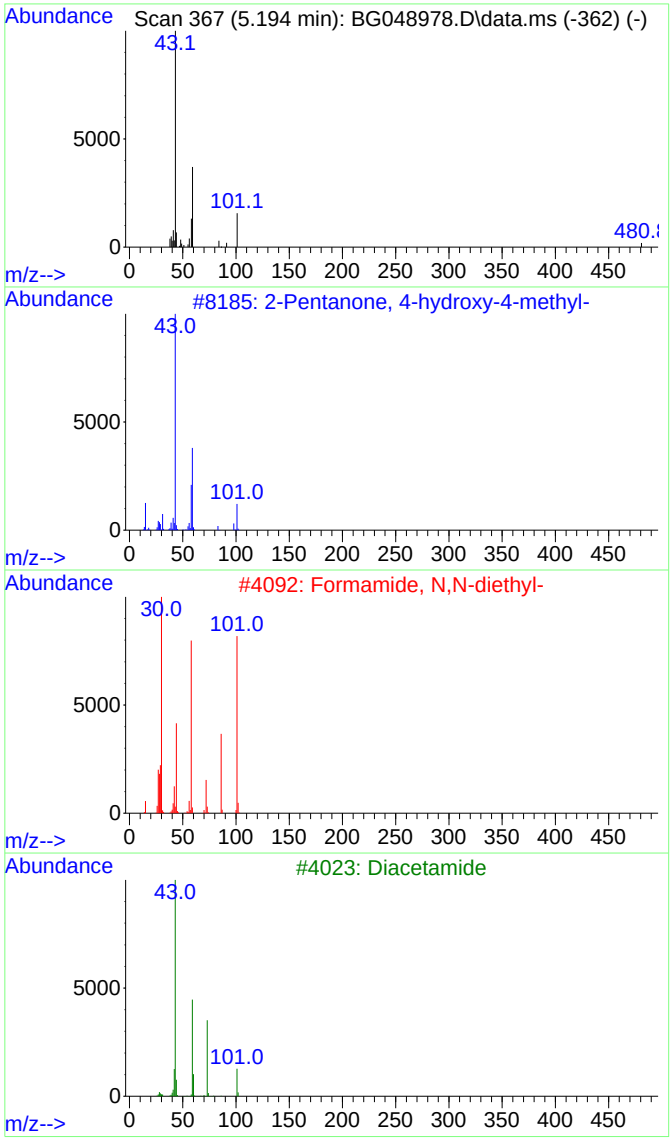
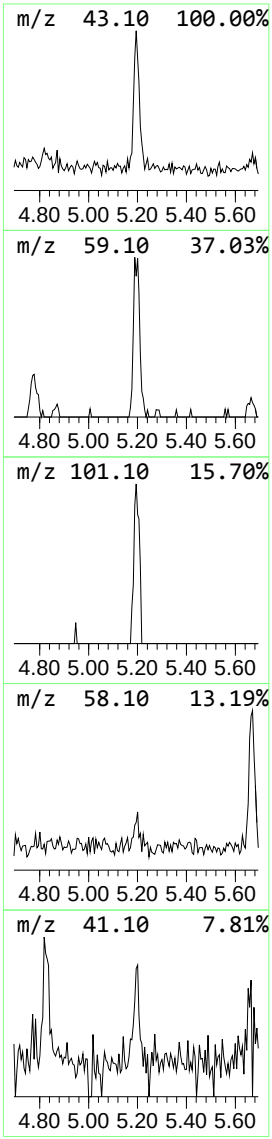
****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.194	3.05 ng	35705	1,4-Dichlorobenzene-d4	8.120

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	33
2	Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9
3	Diacetamide	101	C4H7NO2	000625-77-4	9
4	Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	7





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Sample : M2672-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(28-32)

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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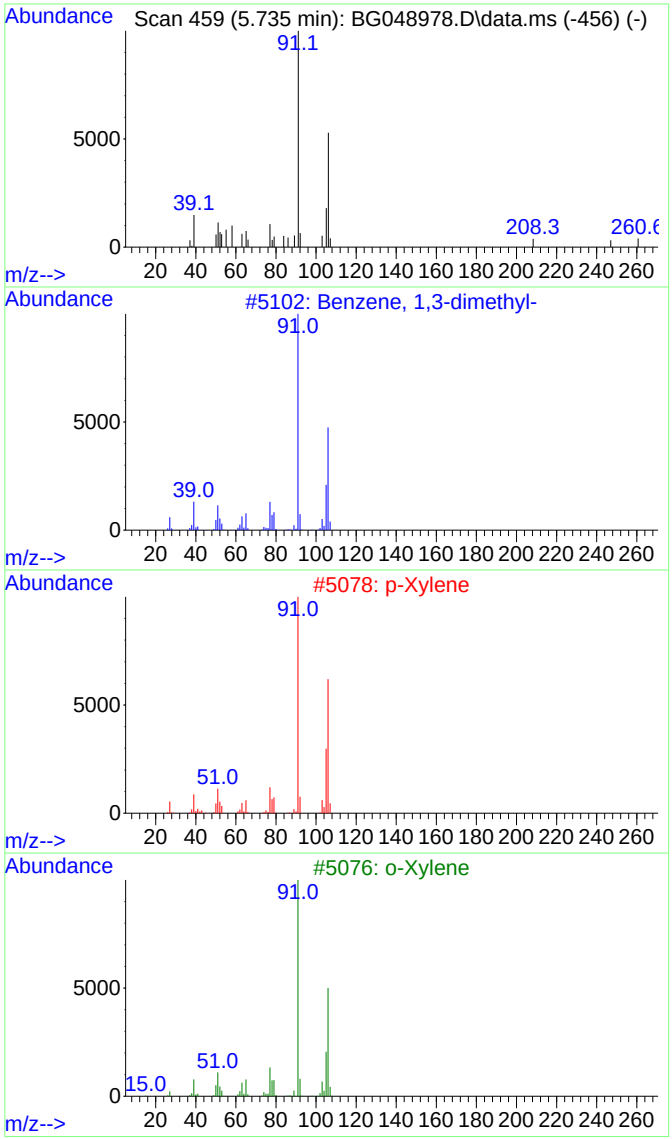
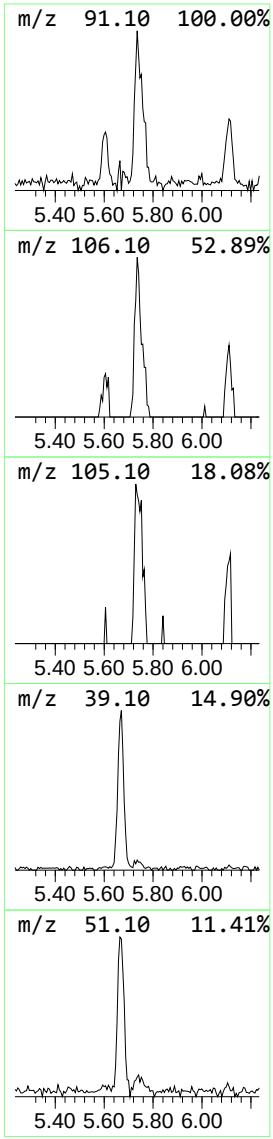
****

Peak Number 4 Benzene, 1,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.735	3.44 ng	40293	1,4-Dichlorobenzene-d4	8.120

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	87
2	p-Xylene	106	C8H10	000106-42-3	83
3	o-Xylene	106	C8H10	000095-47-6	83
4	1,3-Cyclopentadiene, 5-(1-methyl...	106	C8H10	002175-91-9	74
5	Ethylbenzene	106	C8H10	000100-41-4	59





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Operator : CG/JU
Sample : M2672-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(28-32)

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

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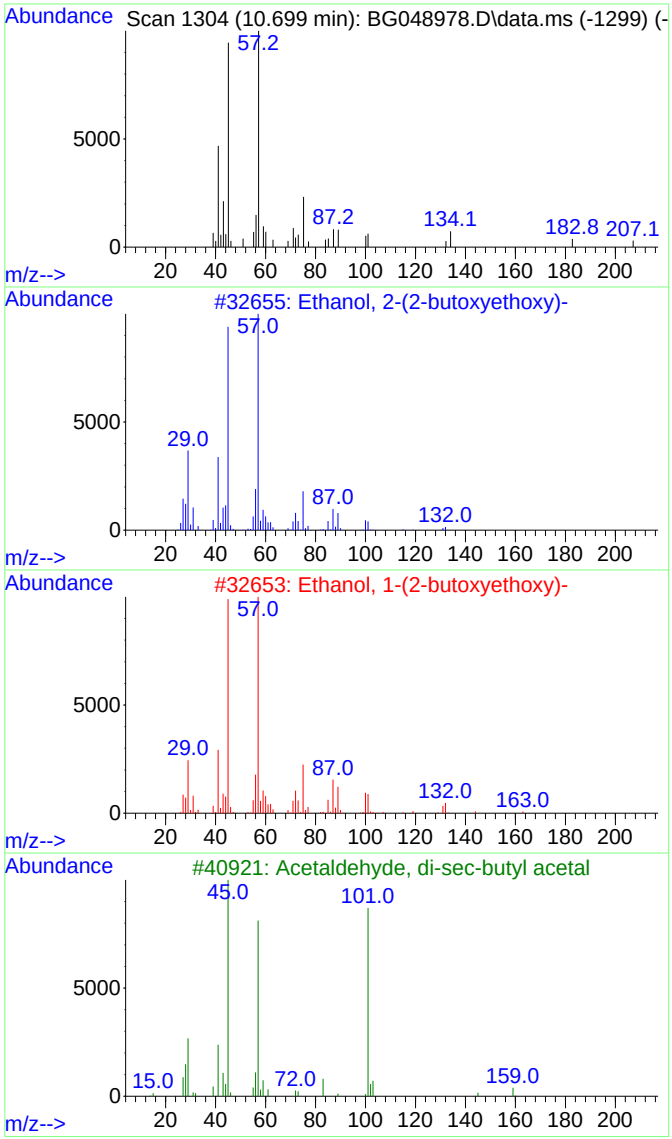
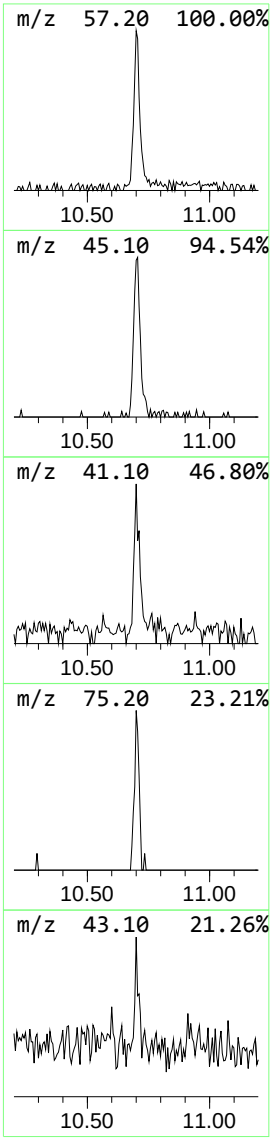
****

Peak Number 5 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.700	2.91 ng	47370	Naphthalene-d8	10.940

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	72
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	56
3	Acetaldehyde, di-sec-butyl acetal	174	C10H22O2	005314-41-0	53
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50
5	Butane, 1,1'-[ethylidenebis(oxy)...	174	C10H22O2	000871-22-7	50





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Misc :
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Instrument : BNA_G
ClientSampleId : 17-B6(28-32)

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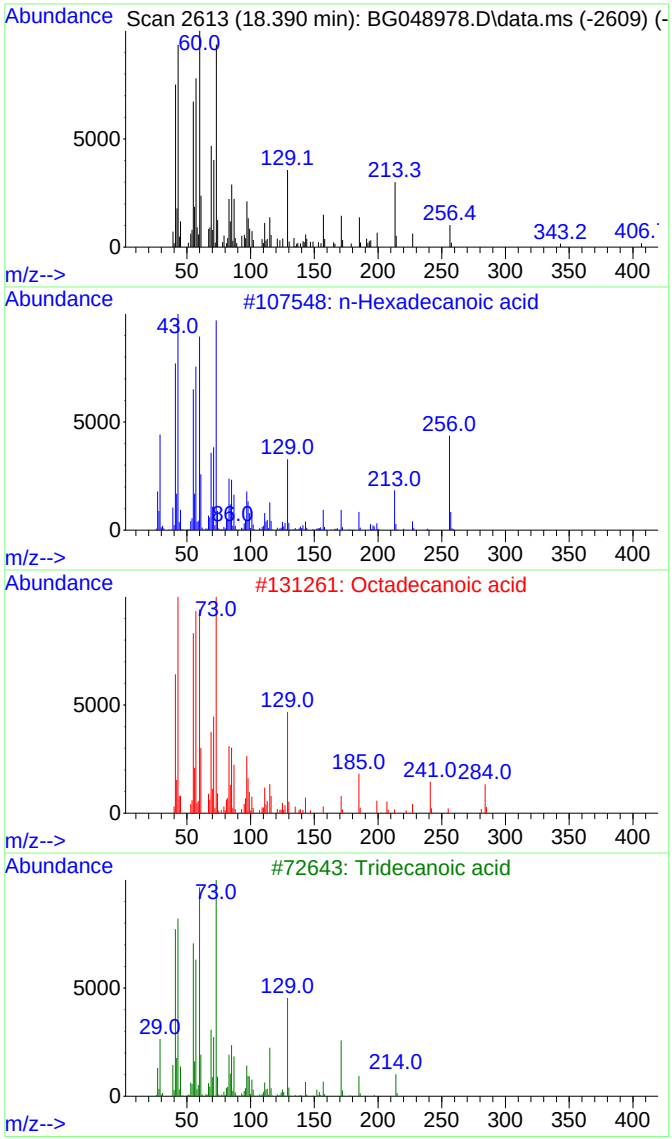
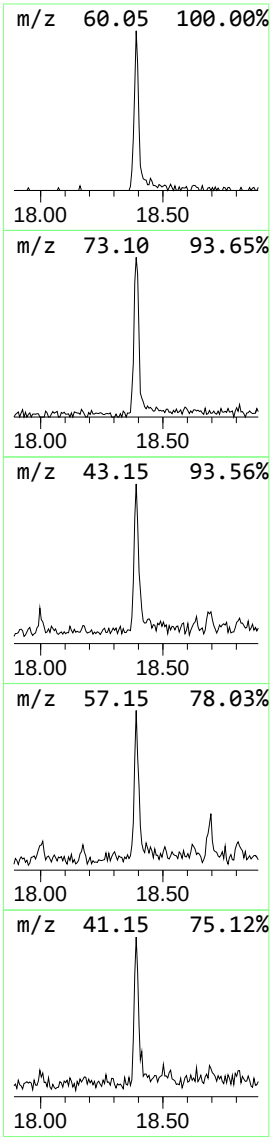
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.390	5.40 ng	158878	Phenanthrene-d10	17.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Octadecanoic acid	284	C18H36O2	000057-11-4	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	80





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Operator : CG/JU
Sample : M2672-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
17-B6(28-32)

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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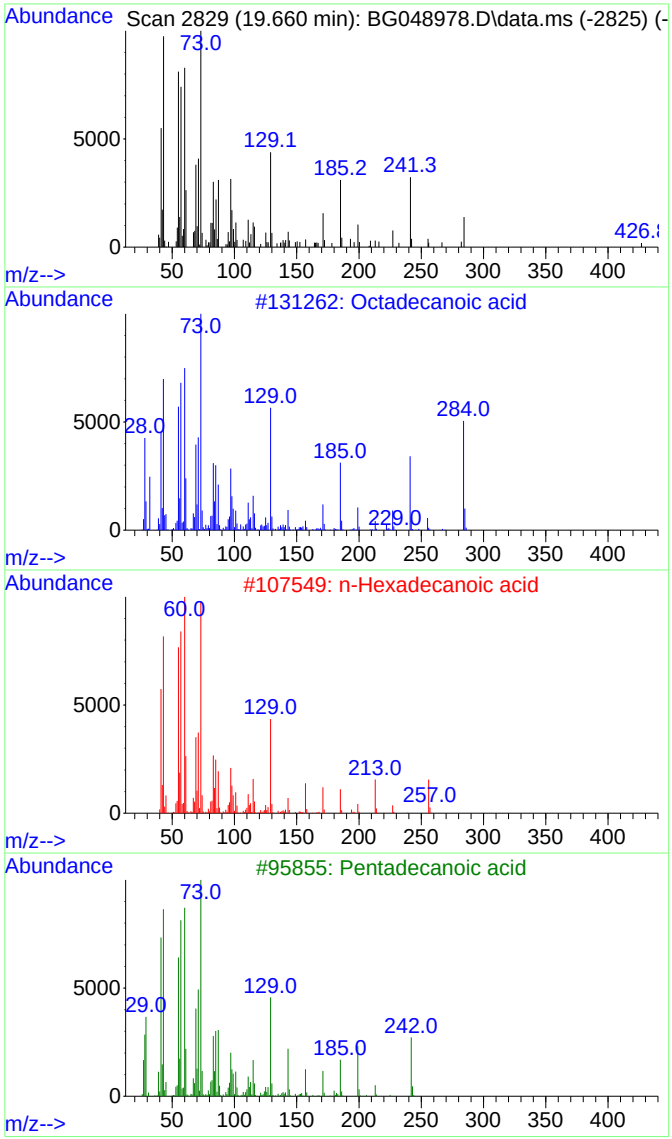
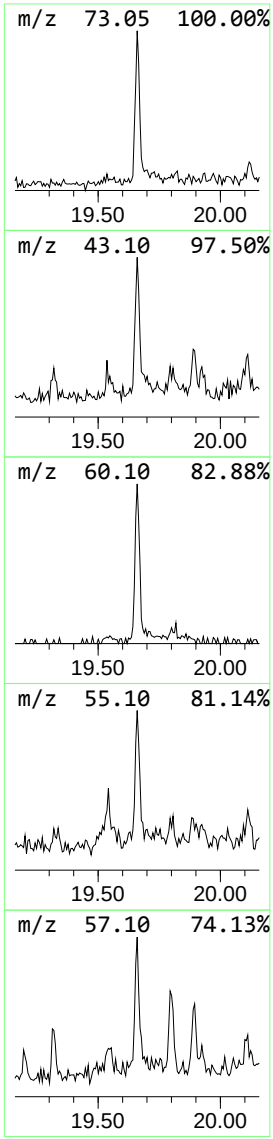
****

Peak Number 7 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.660	3.37 ng	113261	Chrysene-d12	21.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





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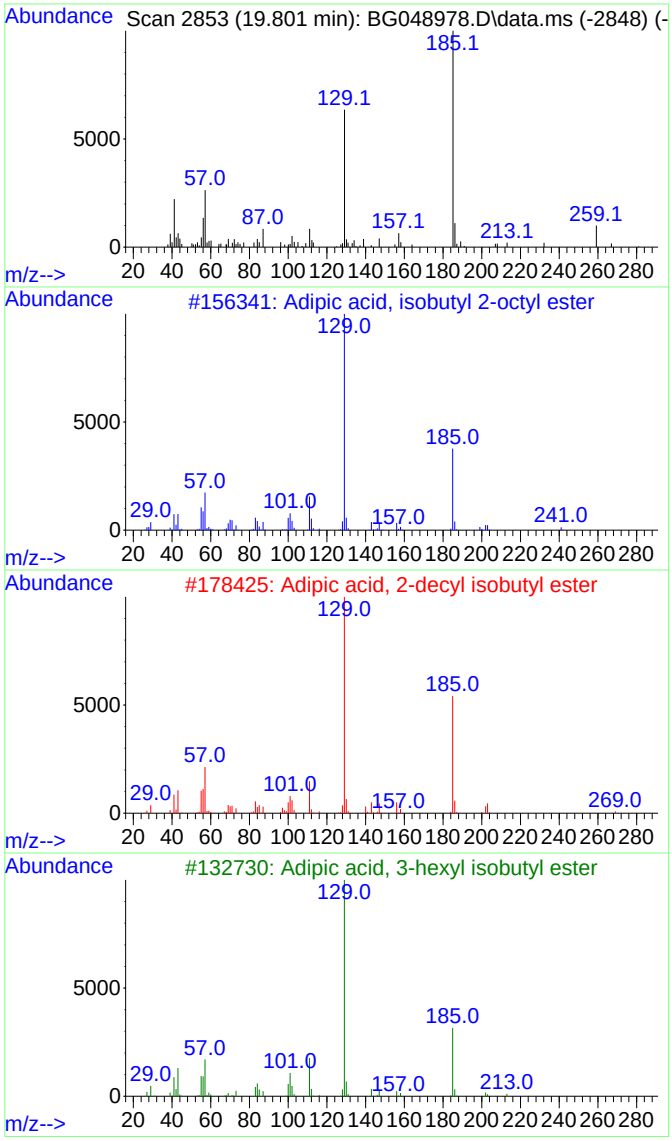
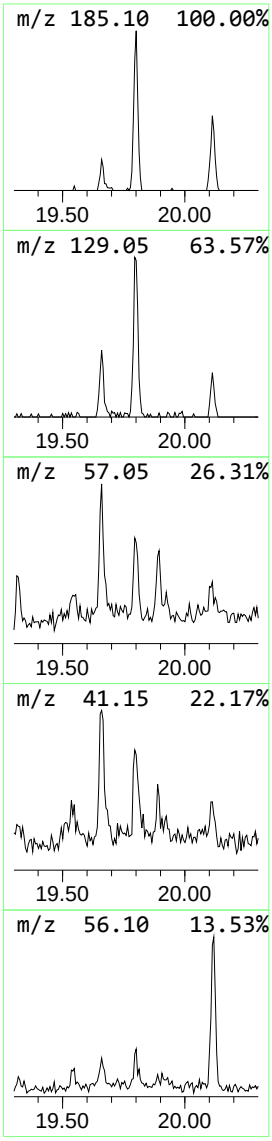
****
Peak Number 8 Adipic acid, isobutyl 2-oct... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.801	2.21 ng	74478	Chrysene-d12	21.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Adipic acid, isobutyl 2-octyl ester	314	C18H34O4	1000324-44-5	72
2	Adipic acid, 2-decyl isobutyl ester	342	C20H38O4	1000353-59-6	72
3	Adipic acid, 3-hexyl isobutyl ester	286	C16H30O4	1000353-62-2	72
4	Dibutyl adipate	258	C14H26O4	000105-99-7	64
5	Adipic acid, butyl isobutyl ester	258	C14H26O4	1000324-09-3	64





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Operator : CG/JU
Sample : M2672-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
17-B6(28-32)

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

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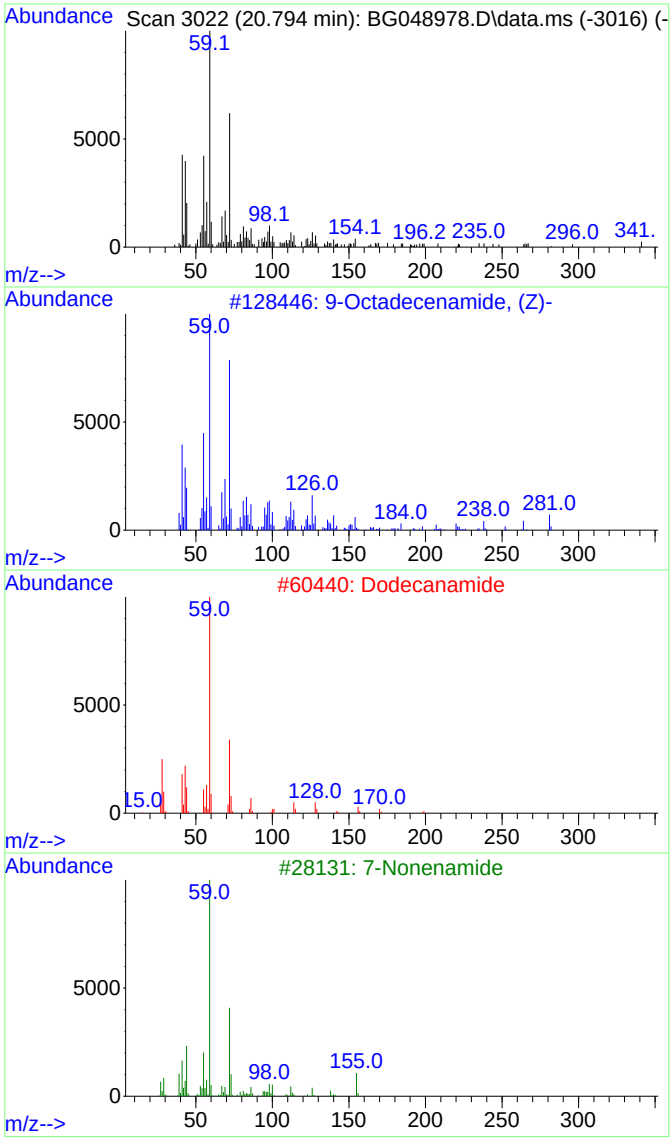
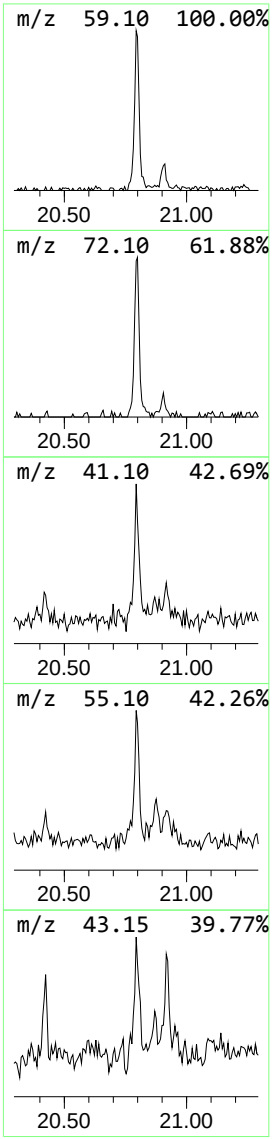
Peak Number 9 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.794	3.82 ng	128418	Chrysene-d12	21.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	83
2	Dodecanamide	199	C12H25NO	001120-16-7	58
3	7-Nonenamide	155	C9H17NO	090949-53-4	50
4	Butanamide, 3,3-dimethyl-	115	C6H13NO	000926-04-5	43
5	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048978.D
Acq On : 15 Jun 2021 15:16
Operator : CG/JU
Sample : M2672-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(28-32)

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

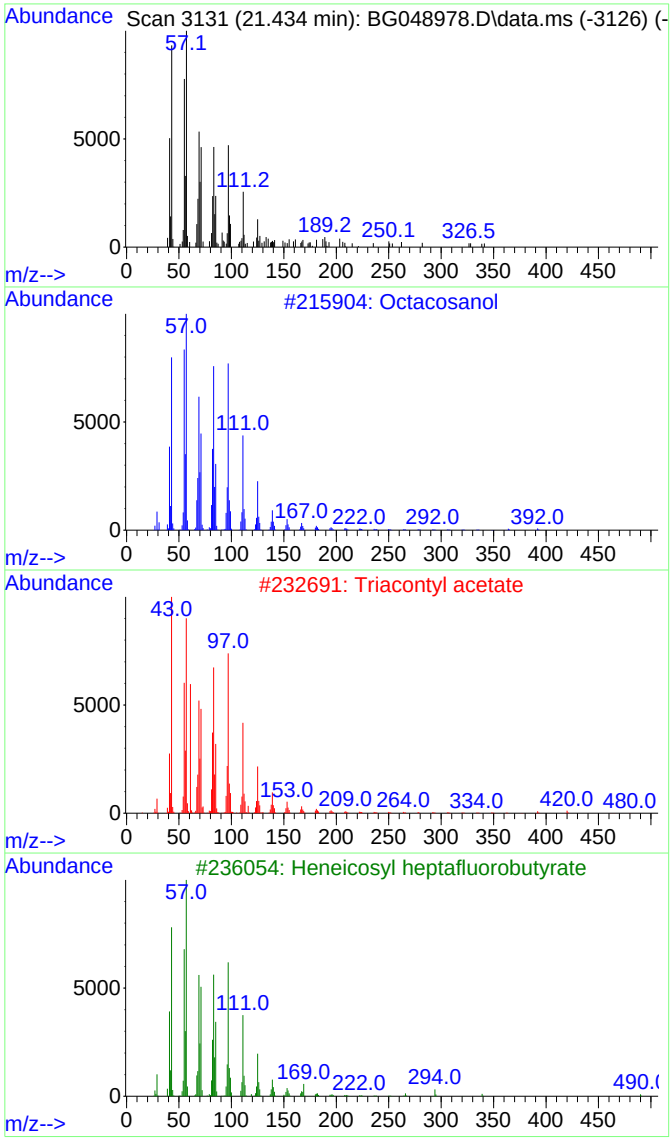
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

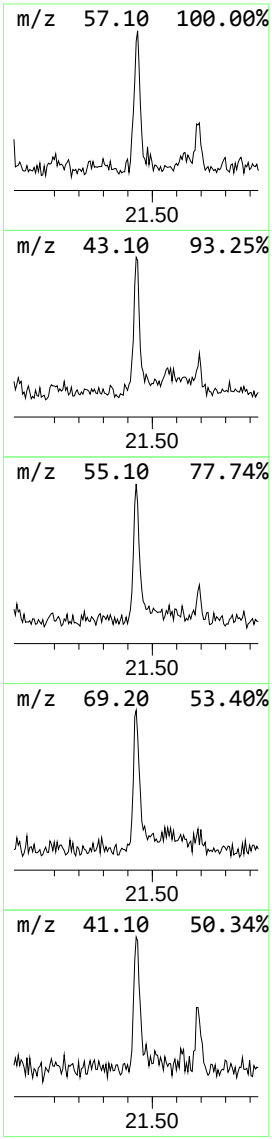
****

Peak Number 10 Octacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.434	4.77 ng	160421	Chrysene-d12	21.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosanol	410	C28H58O	000557-61-9	91
2	Triacontyl acetate	480	C32H64O2	041755-58-2	91
3	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	90
4	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	90
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048978.D
Acq On : 15 Jun 2021 15:16
Operator : CG/JU
Sample : M2672-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(28-32)

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...	3.161	20.4	ng	239256	1	8.120	234469	20.0
Z-1-Methoxy-2-p...	3.285	7.9	ng	92631	1	8.120	234469	20.0
2-Pentanone, 4-...	5.194	3.0	ng	35705	1	8.120	234469	20.0
Benzene, 1,3-di...	5.735	3.4	ng	40293	1	8.120	234469	20.0
Ethanol, 2-(2-b...	10.700	2.9	ng	47370	2	10.940	325096	20.0
n-Hexadecanoic ...	18.390	5.4	ng	158878	4	17.509	588886	20.0
Octadecanoic acid	19.660	3.4	ng	113261	5	21.798	672789	20.0
Adipic acid, is...	19.801	2.2	ng	74478	5	21.798	672789	20.0
9-Octadecenamid...	20.794	3.8	ng	128418	5	21.798	672789	20.0
Octacosanol	21.434	4.8	ng	160421	5	21.798	672789	20.0