LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048983.D
Acq On : 15 Jun 2021 18:41
Operator : CG/JU
Sample : M2672-17
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(72-76)

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: BG048983.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	16	21	33	rVB2	104643	179331	6.11%	1.333%
2	3.285	37	42	49	rVB	65462	99772	3.40%	0.742%
3	5.194	363	367	373	rBV2	21319	32188	1.10%	0.239%
4	5.664	441	447	456	rBV	667763	1100616	37.48%	8.182%
5	5.735	456	459	469	rVB2	24092	51745	1.76%	0.385%
6	7.268	712	720	731	rBV	671172	1194237	40.67%	8.878%
7	8.114	858	864	872	rVB	116023	197554	6.73%	1.469%
8	9.277	1055	1062	1072	rBV	416947	752409	25.62%	5.594%
9	10.699	1296	1304	1312	rBV5	21024	44324	1.51%	0.330%
10	10.934	1336	1344	1353	rBV	142698	260363	8.87%	1.936%
11	13.379	1753	1760	1767	rBV	993109	1563069	53.23%	11.620%
12	14.753	1989	1994	2002	rVB	238352	388488	13.23%	2.888%
13	16.158	2227	2233	2239	rVB	52597	70096	2.39%	0.521%
14	16.246	2240	2248	2263	rVB	918182	1464130	49.86%	10.885%
15	17.503	2456	2462	2469	rBV	340212	535252	18.23%	3.979%
16	17.621	2477	2482	2488	rVB2	77125	109187	3.72%	0.812%
17	18.161	2569	2574	2580	rVB4	46052	66760	2.27%	0.496%
18	18.390	2608	2613	2620	rBV	79152	114245	3.89%	0.849%
19	19.654	2821	2828	2833	rBV	66385	94214	3.21%	0.700%
20	20.112	2899	2906	2912	rBV	2184599	2936469	100.00%	21.830%
21	20.793	3015	3022	3030	rBV	179321	254879	8.68%	1.895%
22	20.870	3032	3035	3038	rVV2	30338	34891	1.19%	0.259%
23	21.434	3125	3131	3140	rBV3	83847	157630	5.37%	1.172%
24	21.686	3169	3174	3182	rVB	57458	93180	3.17%	0.693%
25	21.798	3186	3193	3201	rVV	380508	647275	22.04%	4.812%
26	22.004	3224	3228	3233	rBV3	24543	37595	1.28%	0.279%
27	22.638	3332	3336	3346	rVB7	35062	74842	2.55%	0.556%
28	23.026	3396	3402	3406	rBV3	35277	64281	2.19%	0.478%
29	23.326	3448	3453	3466	rVB4	83854	205083	6.98%	1.525%
30	25.130	3750	3760	3770	rBV2	210539	627148	21.36%	4.662%

Sum of corrected areas: 13451253

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Misc :
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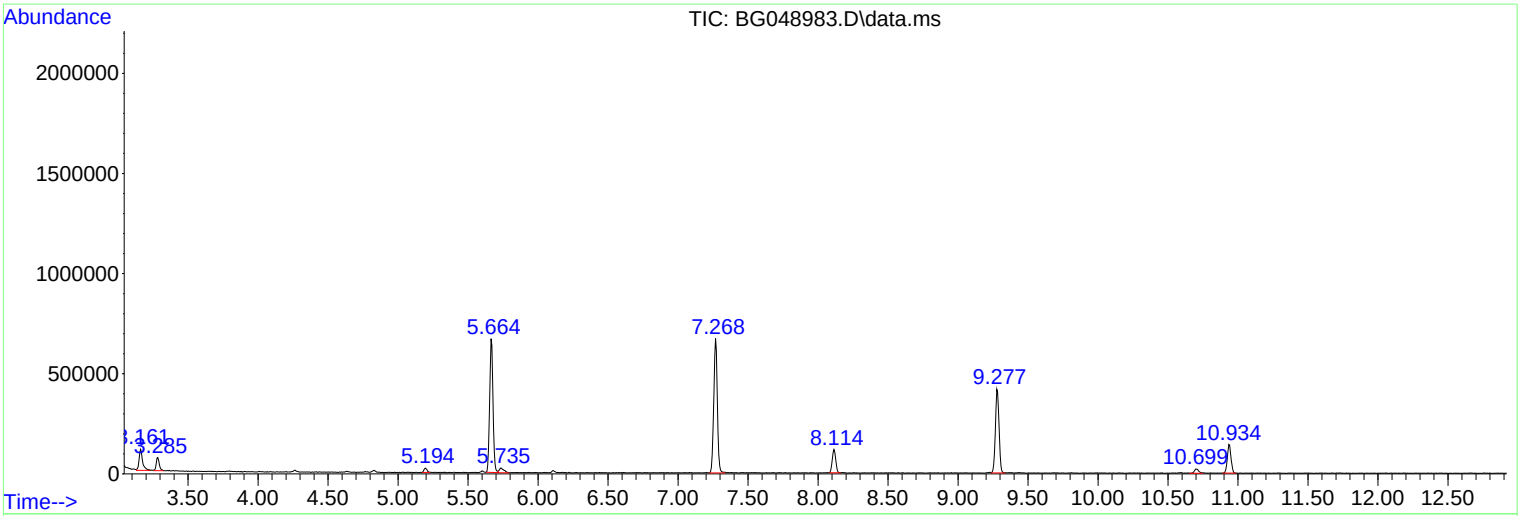
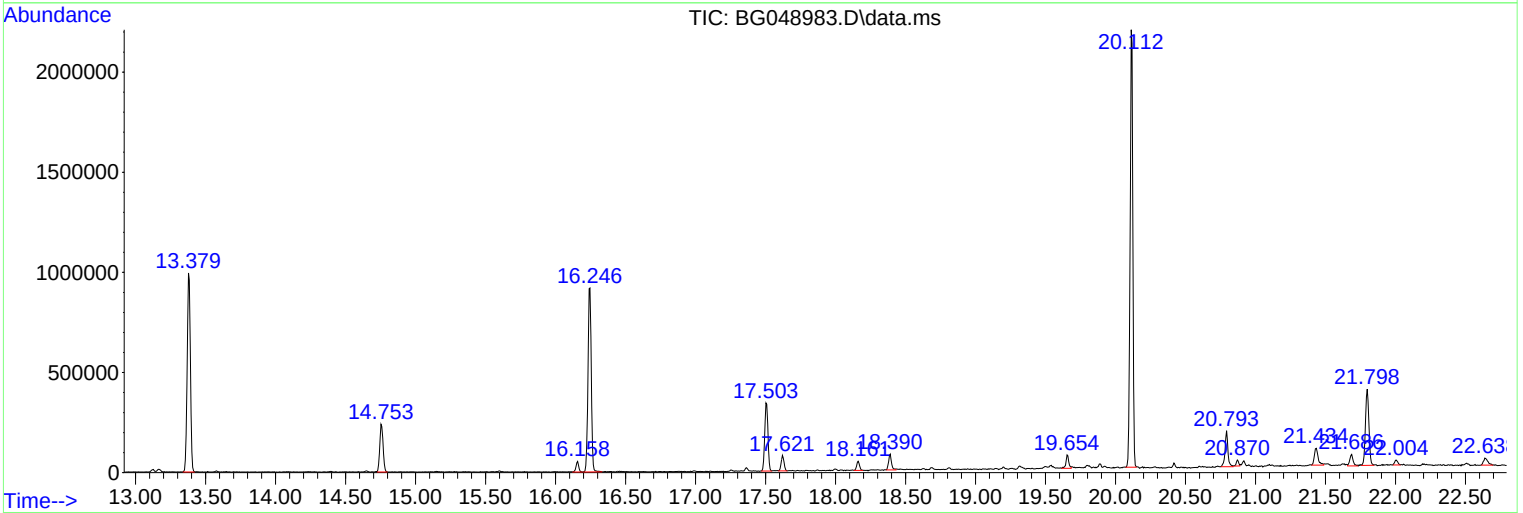
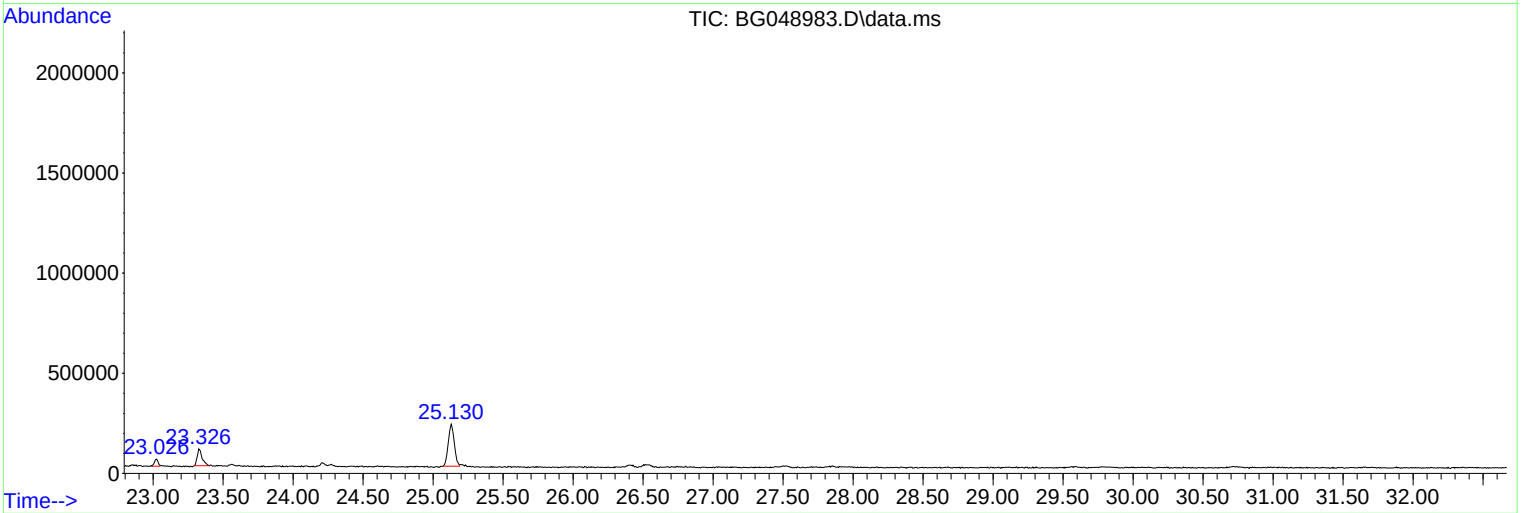
Instrument :
BNA_G
ClientSampleId :
17-B6(72-76)

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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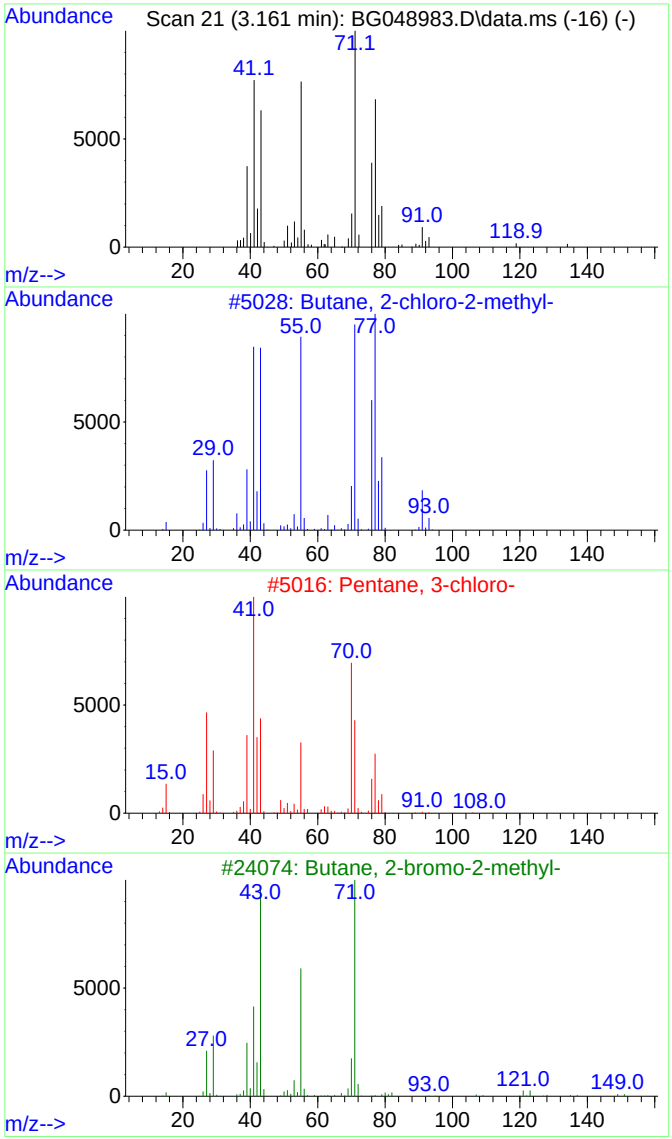
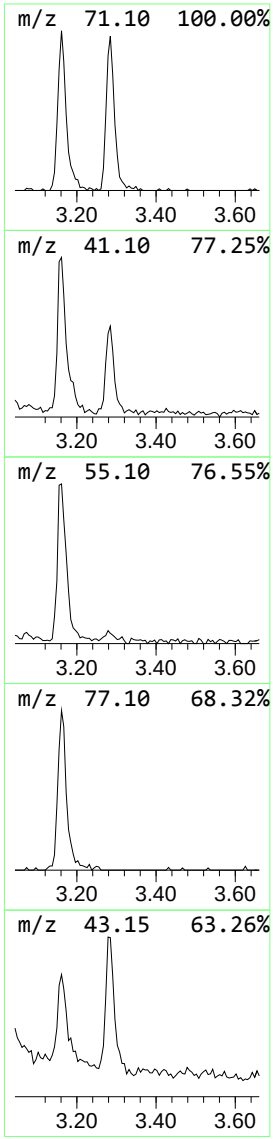
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.161	18.16 ng	179331	1,4-Dichlorobenzene-d4	8.114

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-chloro-2-methyl-	106	C5H11Cl	000594-36-5	78
2	Pentane, 3-chloro-	106	C5H11Cl	000616-20-6	38
3	Butane, 2-bromo-2-methyl-	150	C5H11Br	000507-36-8	32
4	4,4-Dimethyl-1-hexene	112	C8H16	001647-08-1	23
5	Borinic acid, diethyl-, methyl e...	100	C5H13BO	007397-46-8	22





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Operator : CG/JU
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Misc :
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Instrument : BNA_G
ClientSampleId : 17-B6(72-76)

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

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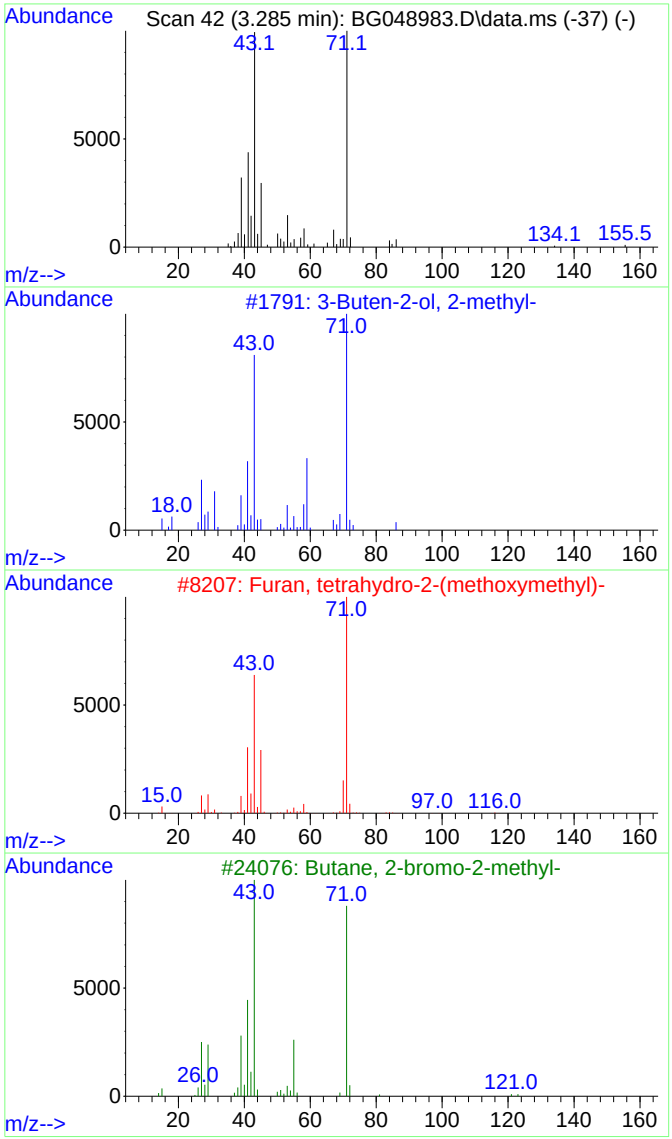
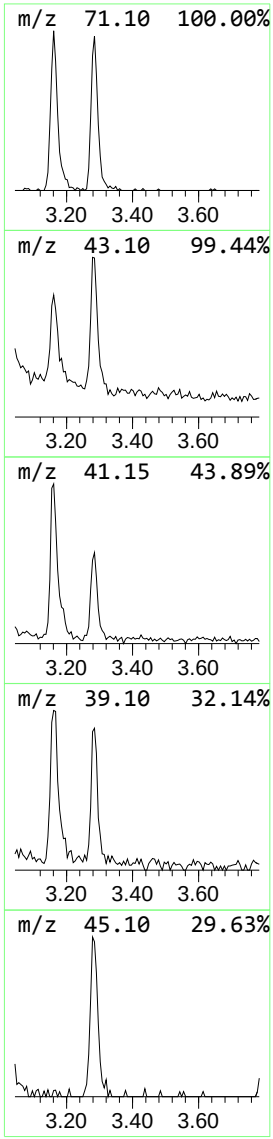
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.285	10.10 ng	99772	1,4-Dichlorobenzene-d4	8.114

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	64
2	Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	59
3	Butane, 2-bromo-2-methyl-	150	C5H11Br	000507-36-8	59
4	2-Furanmethanol, tetrahydro-	102	C5H10O2	000097-99-4	50
5	Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	50





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Operator : CG/JU
Sample : M2672-17
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(72-76)

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

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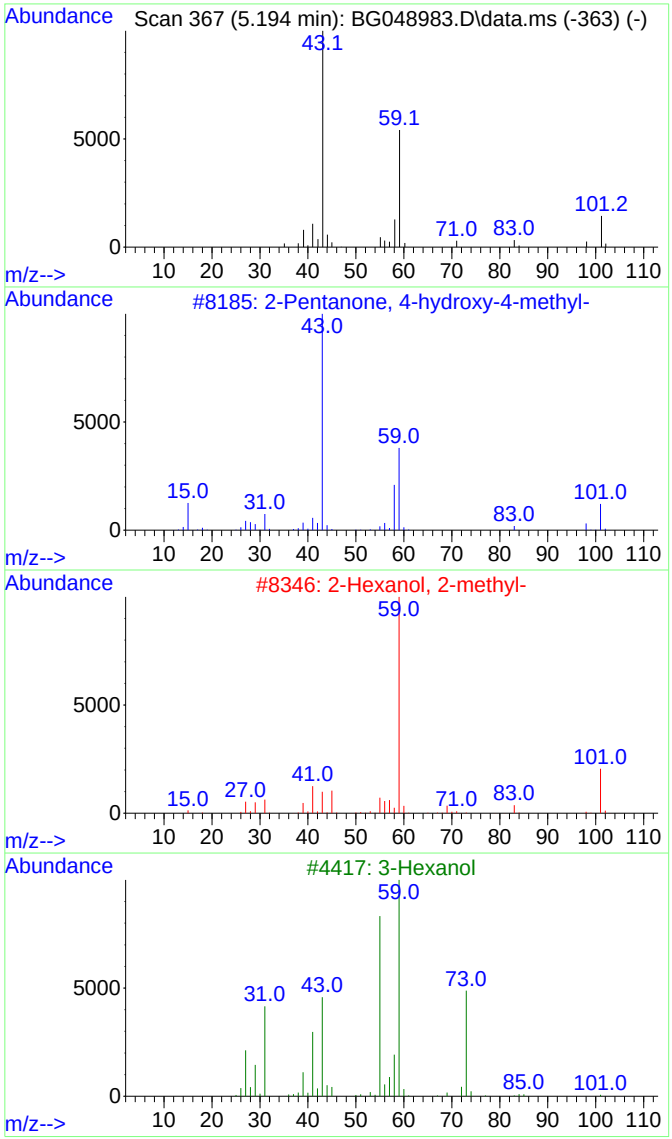
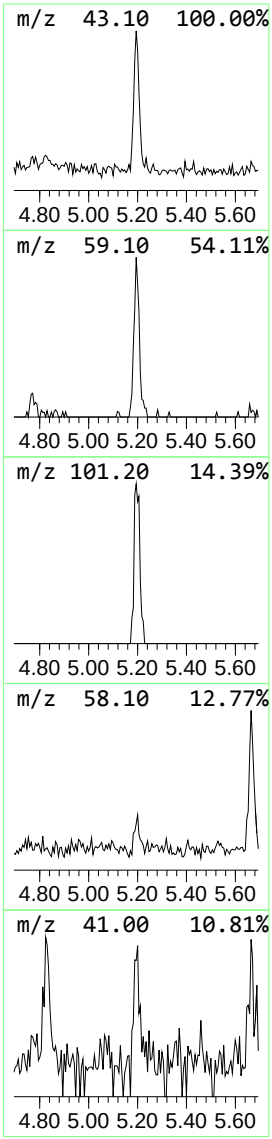
****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.194	3.26 ng	32188	1,4-Dichlorobenzene-d4	8.114

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	47
3	3-Hexanol	102	C6H14O	000623-37-0	38
4	3-Octanol	130	C8H18O	000589-98-0	28
5	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	25





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Instrument : BNA_G
ClientSampleId : 17-B6(72-76)

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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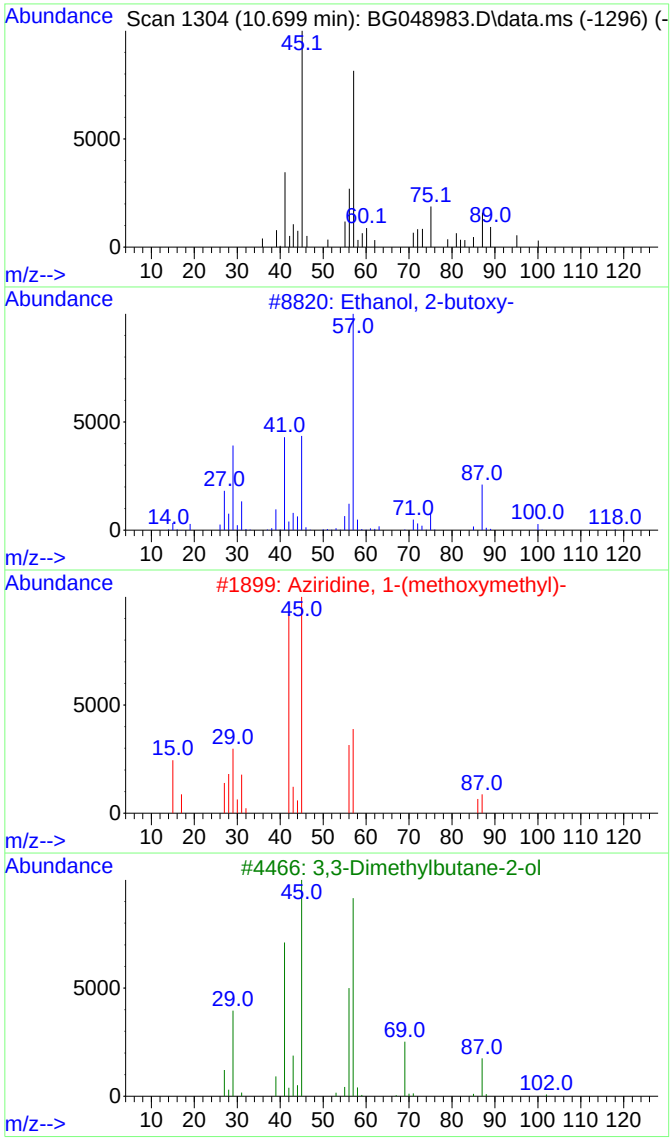
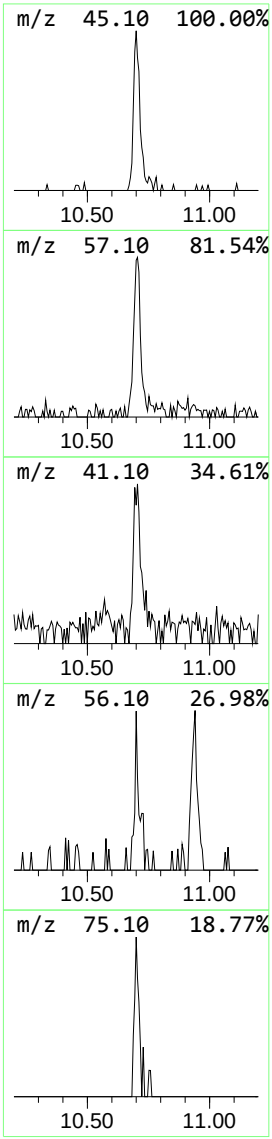
****

Peak Number 5 unknown10.699 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.699	3.40 ng	44324	Naphthalene-d8	10.940

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	42
2	Aziridine, 1-(methoxymethyl)-	87	C4H9NO	001497-83-2	40
3	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	33
4	1-Methoxy-3-methyl-3-butene	100	C6H12O	034752-58-4	32
5	Ethanol, 2-[2-(2-propenyloxy)eth...	146	C7H14O3	015075-50-0	28





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Instrument : BNA_G
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
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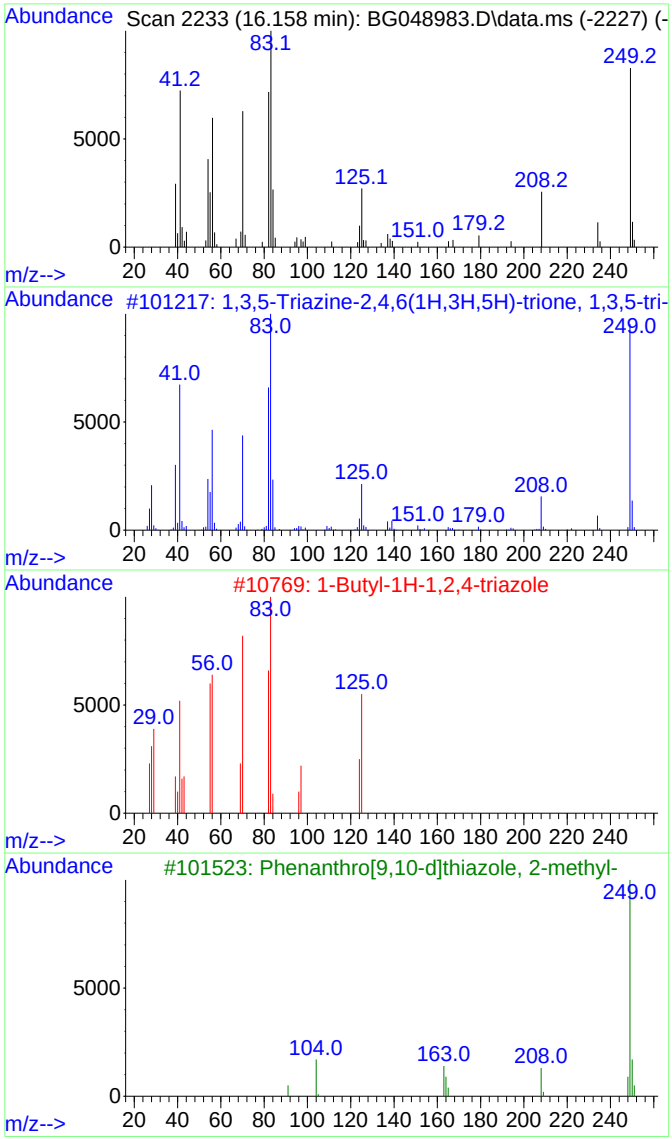
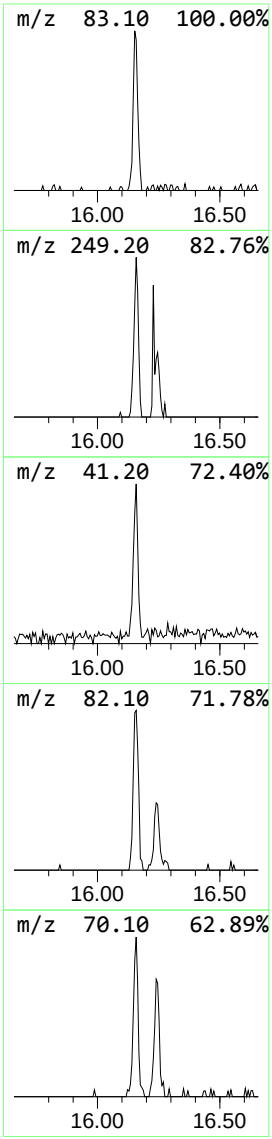
****
Peak Number 6 1,3,5-Triazine-2,4,6(1H,3H,... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.158	2.62 ng	70096	Phenanthrene-d10	17.503

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	94
2	1-Butyl-1H-1,2,4-triazole	125	C6H11N3	006086-22-2	47
3	Phenanthro[9,10-d]thiazole, 2-me...	249	C16H11NS	021639-90-7	40
4	8,8-Dimethylspiro(4.6)undecane-6...	208	C13H20O2	068181-81-7	38
5	Azetidine, 2-methyl-1-[3,3,3-tri...	249	C8H9F6NO	050837-79-1	25





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
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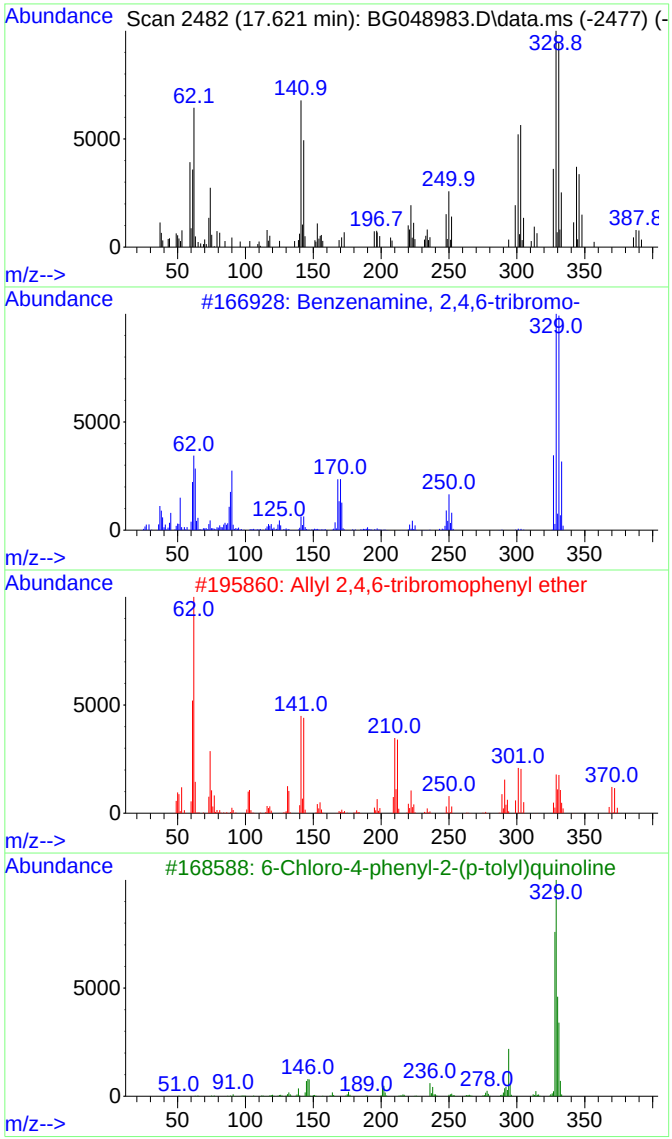
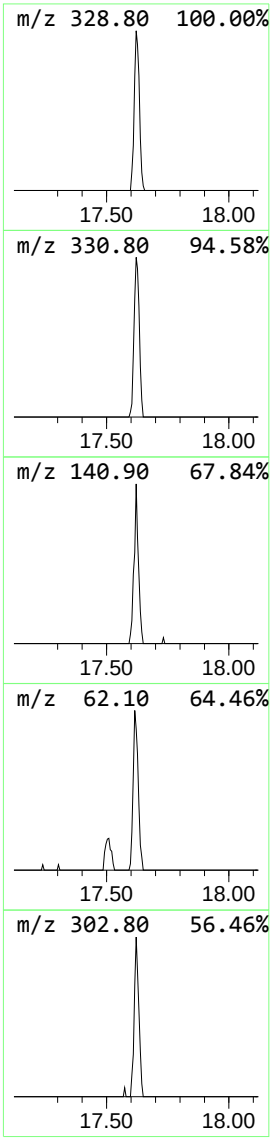
Peak Number 7 Benzenamine, 2,4,6-tribromo- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.621	4.08 ng	109187	Phenanthrene-d10	17.503

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenamine, 2,4,6-tribromo-	327	C6H4Br3N	000147-82-0	70
2	Allyl 2,4,6-tribromophenyl ether	368	C9H7Br3O	003278-89-5	12
3	6-Chloro-4-phenyl-2-(p-tolyl)qui...	329	C22H16ClN	021923-41-1	9
4	4-(2-Methyl-1-cyclohexenyl)-tran...	344	C17H20N4O4	1000243-16-2	9
5	2H,8H-Benzo[1,2-b:5,4-b']dipyran...	344	C20H24O5	026535-35-3	9





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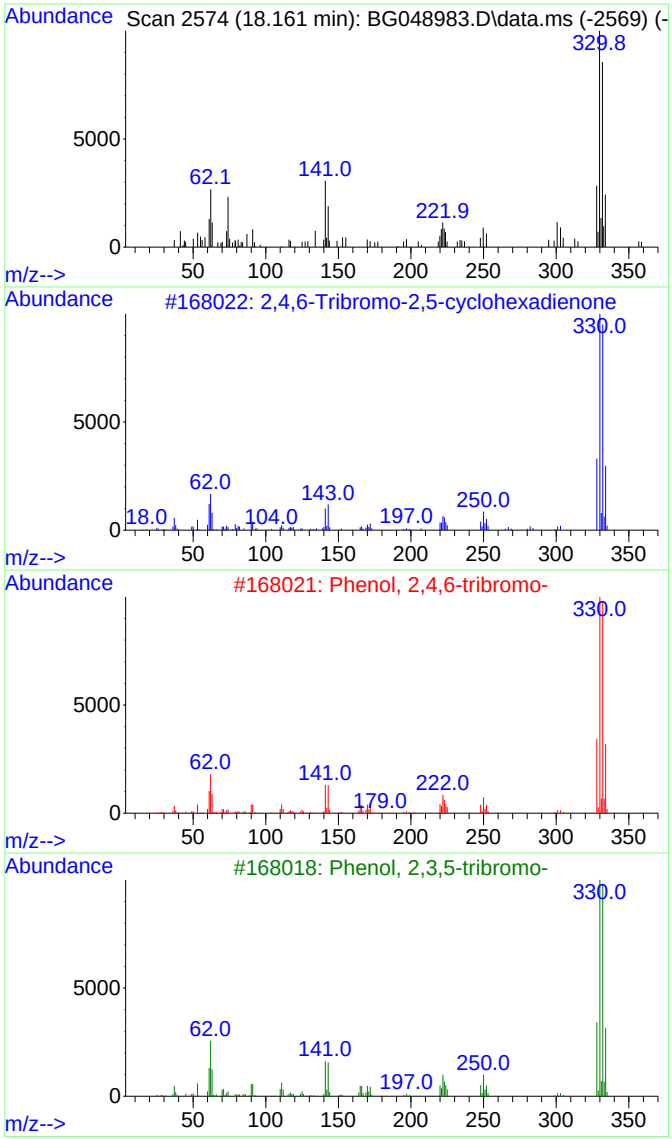
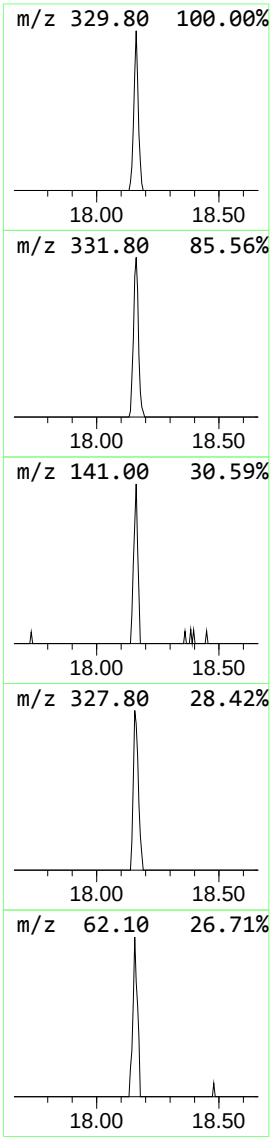
Peak Number 8 2,4,6-Tribromo-2,5-cyclohex... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.161	2.49 ng	66760	Phenanthrene-d10	17.503

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,6-Tribromo-2,5-cyclohexadienone	328	C6H3Br3O	020244-61-5	96
2	Phenol, 2,4,6-tribromo-	328	C6H3Br3O	000118-79-6	96
3	Phenol, 2,3,5-tribromo-	328	C6H3Br3O	057383-81-0	58
4	2-Bromo-4-chloro-5,8-dimethoxy-3...	330	C13H12BrClO3	104506-11-8	38
5	7-Bromo-2,3-dihydro-5-phenyl-1H-...	330	C15H11BrN2S	034099-70-2	23





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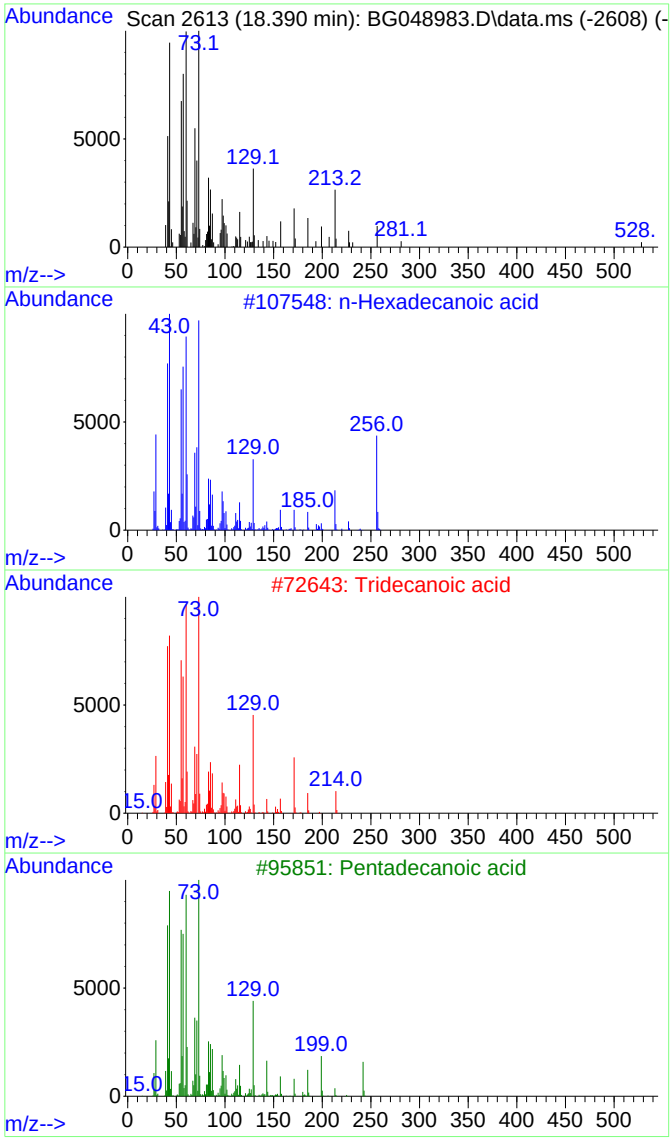
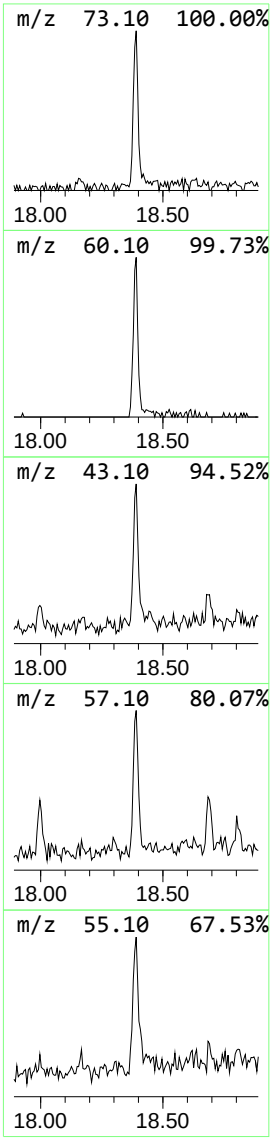
Peak Number 9 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.390	4.27 ng	114245	Phenanthrene-d10	17.503

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Octadecanoic acid	284	C18H36O2	000057-11-4	70
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





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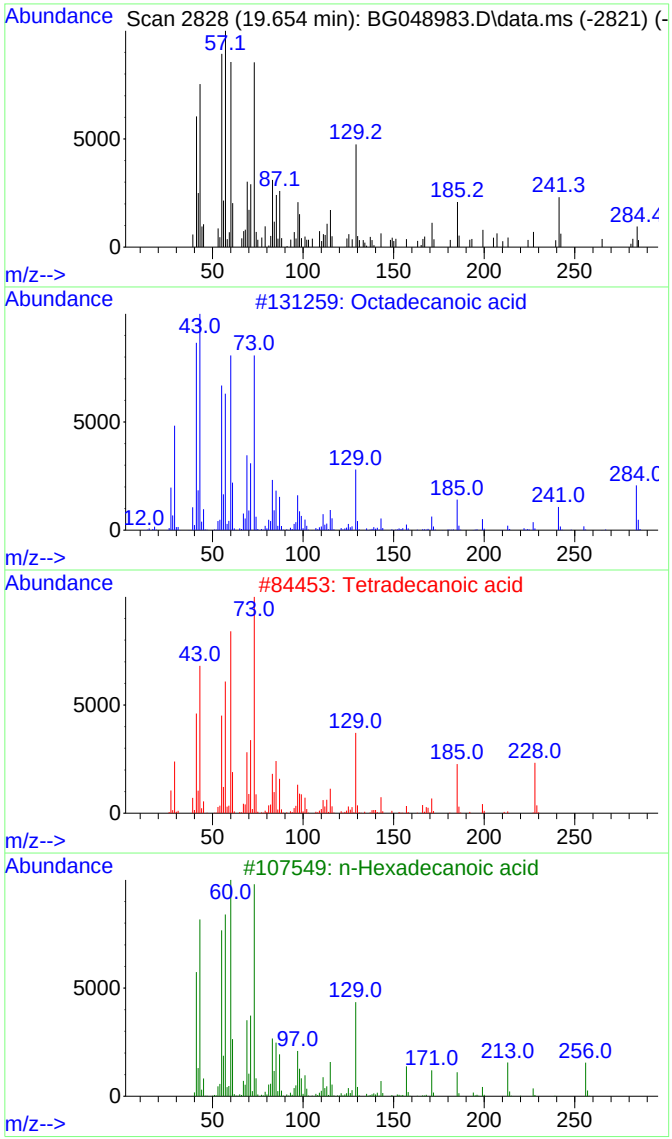
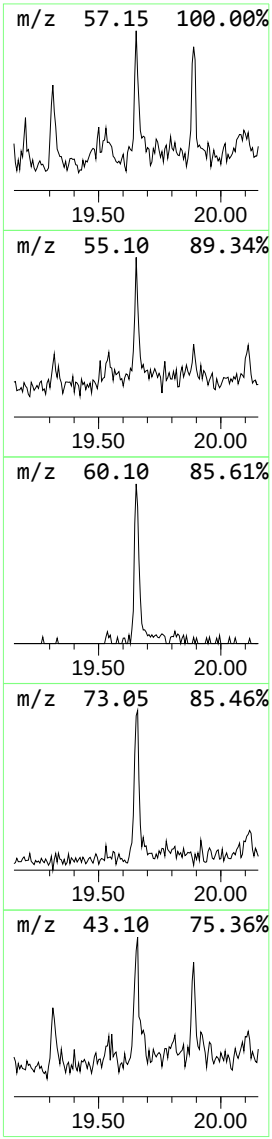
Peak Number 10 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.654	2.91 ng	94214	Chrysene-d12	21.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048983.D
Acq On : 15 Jun 2021 18:41
Operator : CG/JU
Sample : M2672-17
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(72-76)

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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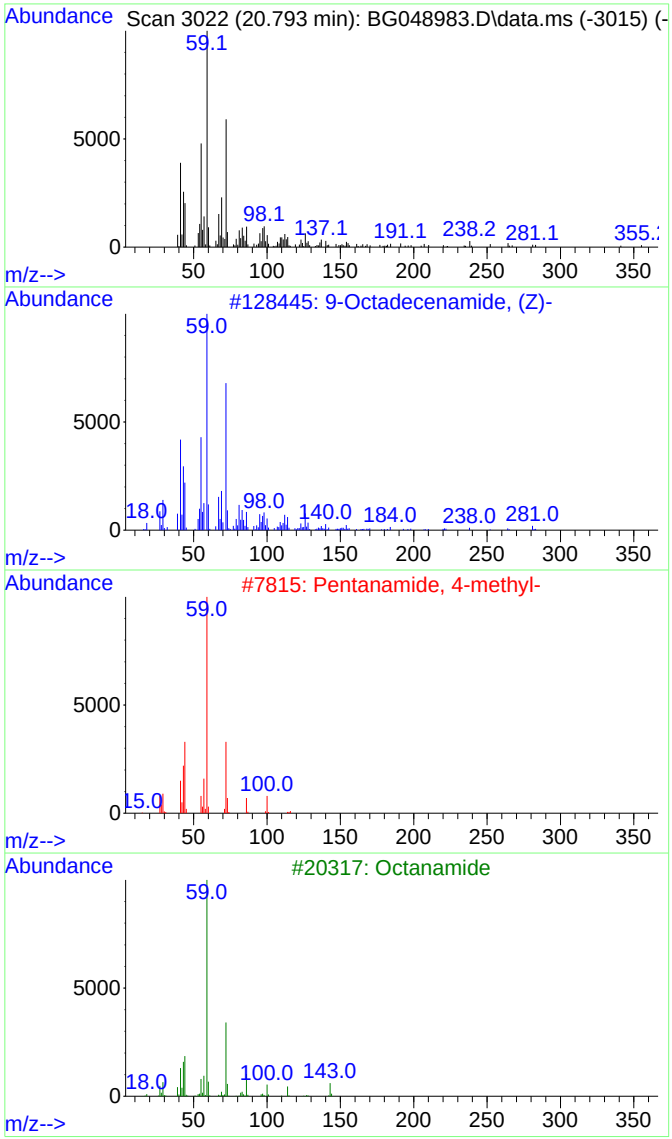
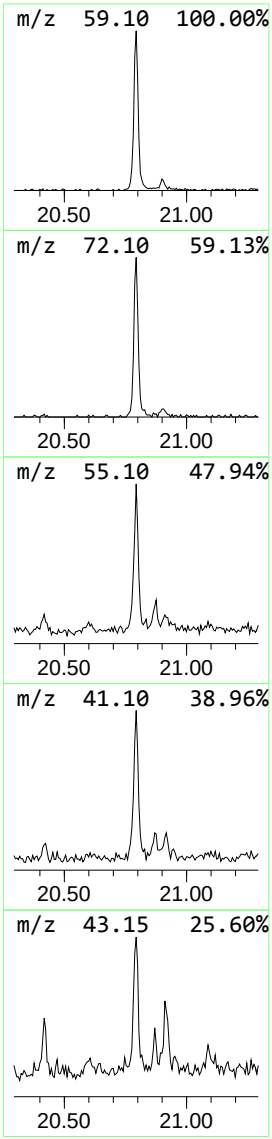
Peak Number 11 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.793	7.88 ng	254879	Chrysene-d12	21.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	95
2	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	64
3	Octanamide	143	C8H17NO	000629-01-6	64
4	Nonanamide	157	C9H19NO	001120-07-6	53
5	Diazene, [1-(2,2-dimethylhydrazi...	172	C8H20N4	061940-94-1	47





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Data File : BG048983.D
Acq On : 15 Jun 2021 18:41
Operator : CG/JU
Sample : M2672-17
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(72-76)

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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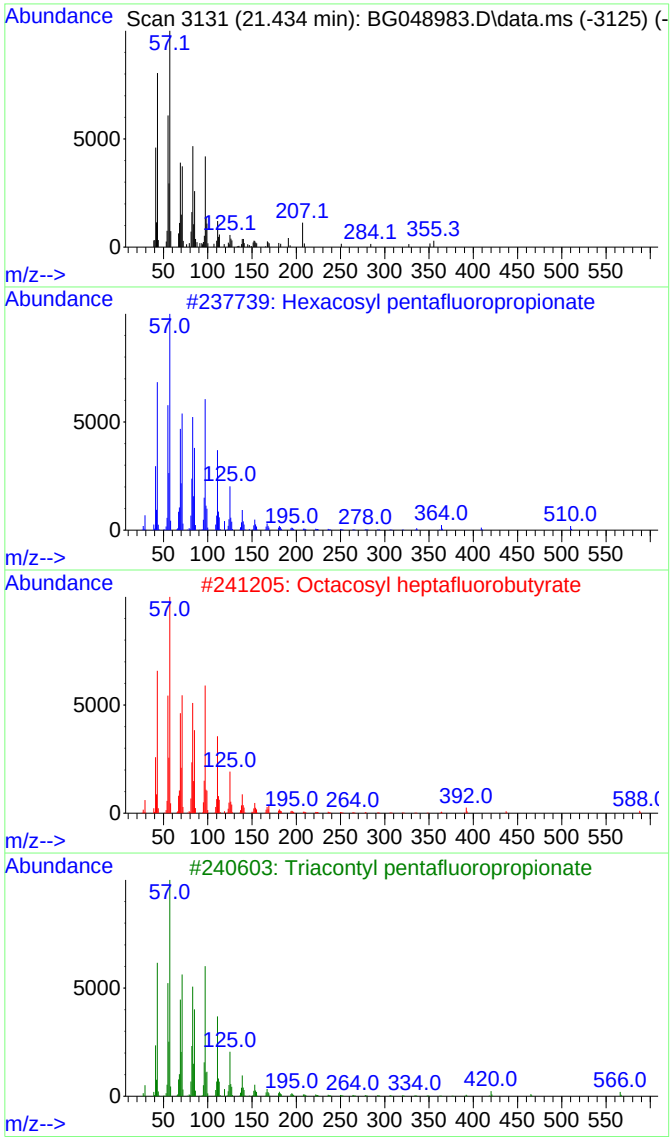
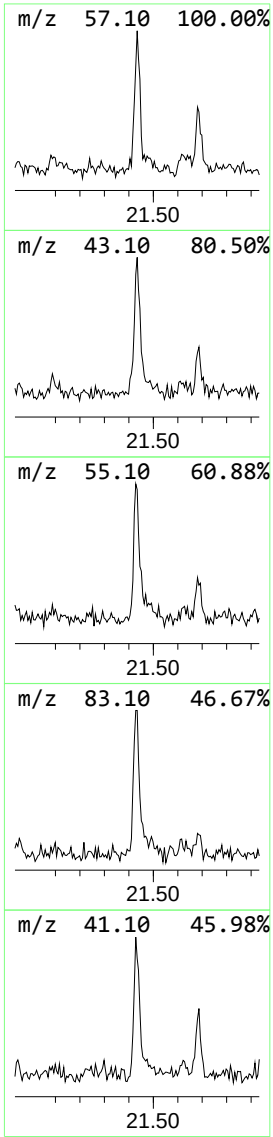
Peak Number 12 Hexacosyl pentafluoropropio... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.434	4.87 ng	157630	Chrysene-d12	21.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosyl pentafluoropropionate	528	C29H53F5O2	1000351-81-2	86
2	Octacosyl heptafluorobutyrate	606	C32H57F7O2	1000351-83-6	86
3	Triacontyl pentafluoropropionate	584	C33H61F5O2	1000351-80-0	80
4	Hexacosyl trifluoroacetate	478	C28H53F3O2	1000351-75-0	80
5	Dotriacontyl heptafluorobutyrate	662	C36H65F7O2	1000351-84-2	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048983.D
Acq On : 15 Jun 2021 18:41
Operator : CG/JU
Sample : M2672-17
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
17-B6(72-76)

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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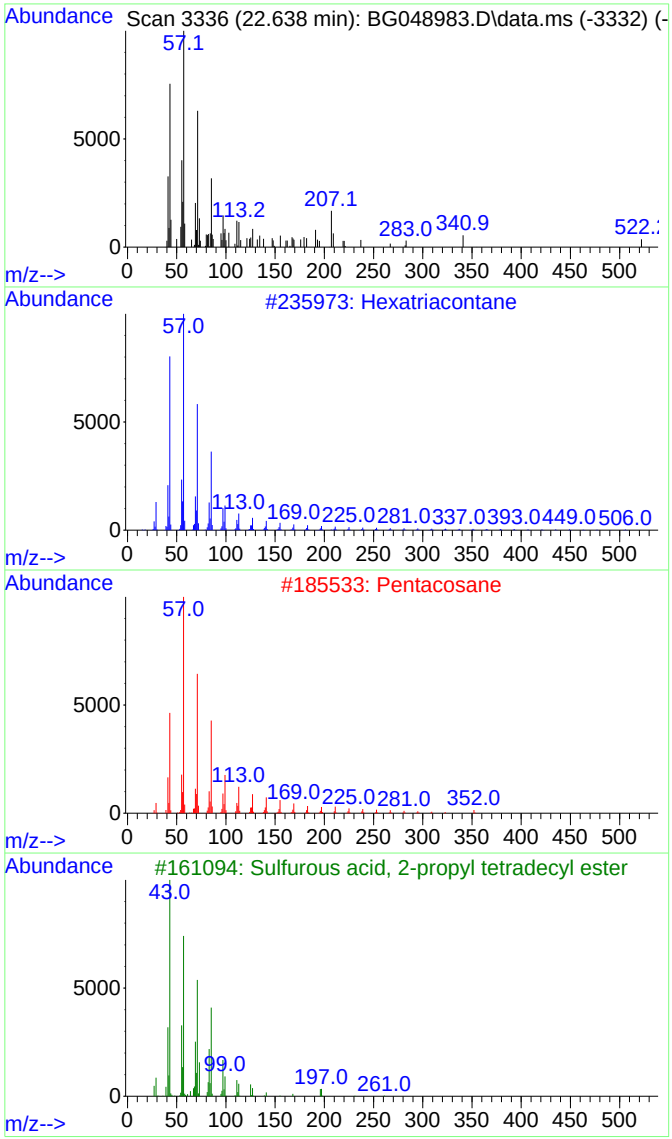
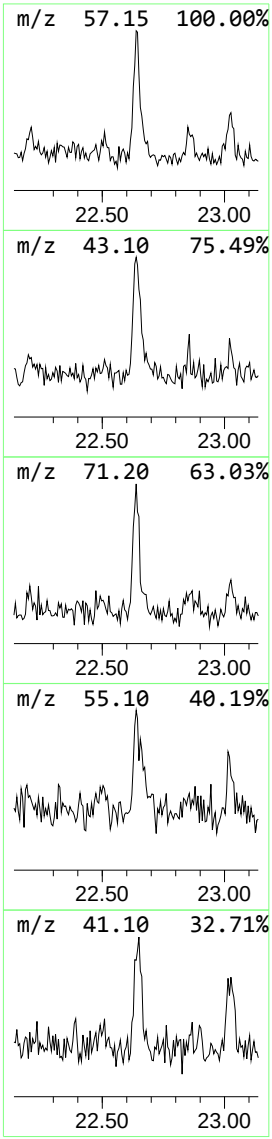
Peak Number 13 Hexatriacontane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.638	2.31 ng	74842	Chrysene-d12	21.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexatriacontane	507	C36H74	000630-06-8	59
2	Pentacosane	352	C25H52	000629-99-2	59
3	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	53
4	2-methylhexacosane	380	C27H56	1000376-72-7	53
5	Docosane	310	C22H46	000629-97-0	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048983.D
Acq On : 15 Jun 2021 18:41
Operator : CG/JU
Sample : M2672-17
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
17-B6(72-76)

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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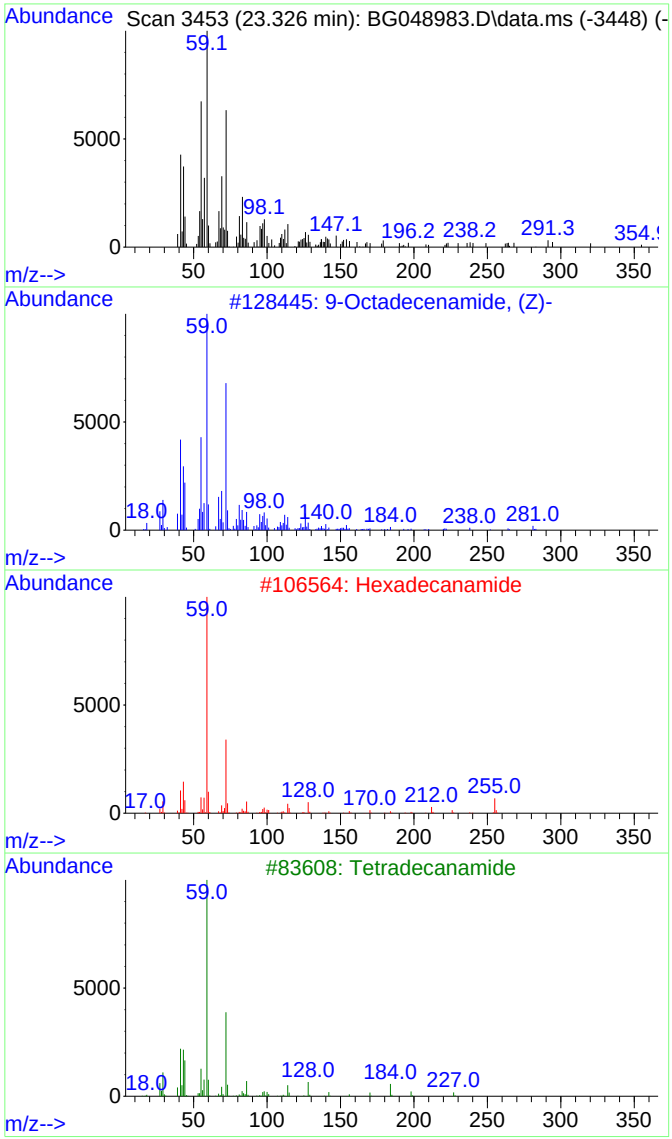
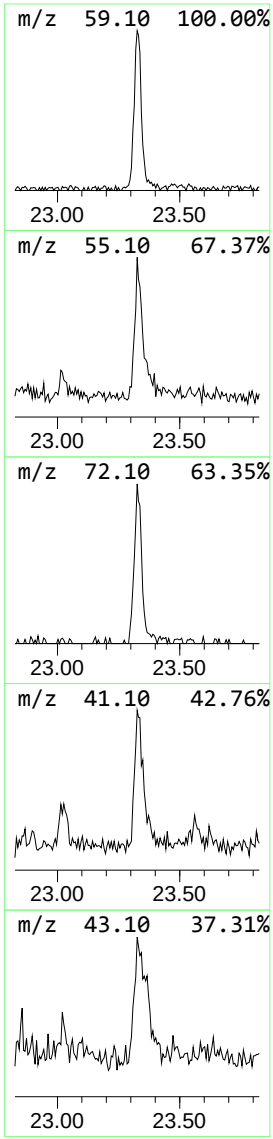
Peak Number 14 Hexadecanamide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.326	6.34 ng	205083	Chrysene-d12	21.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	80
2	Hexadecanamide	255	C16H33NO	000629-54-9	50
3	Tetradecanamide	227	C14H29NO	000638-58-4	50
4	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	50
5	Dodecanamide	199	C12H25NO	001120-16-7	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048983.D
Acq On : 15 Jun 2021 18:41
Operator : CG/JU
Sample : M2672-17
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(72-76)

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	18.2	ng	179331	1	8.114	197554	20.0
3-Buten-2-ol, 2...	3.285	10.1	ng	99772	1	8.114	197554	20.0
2-Pentanone, 4-...	5.194	3.3	ng	32188	1	8.114	197554	20.0
unknown10.699	10.699	3.4	ng	44324	2	10.940	260363	20.0
1,3,5-Triazine-...	16.158	2.6	ng	70096	4	17.503	535252	20.0
Benzenamine, 2,...	17.621	4.1	ng	109187	4	17.503	535252	20.0
2,4,6-Tribromo-...	18.161	2.5	ng	66760	4	17.503	535252	20.0
n-Hexadecanoic ...	18.390	4.3	ng	114245	4	17.503	535252	20.0
Octadecanoic acid	19.654	2.9	ng	94214	5	21.798	647275	20.0
9-Octadecenamid...	20.793	7.9	ng	254879	5	21.798	647275	20.0
Hexacosyl penta...	21.434	4.9	ng	157630	5	21.798	647275	20.0
Hexatriacontane	22.638	2.3	ng	74842	5	21.798	647275	20.0
Hexadecanamide	23.326	6.3	ng	205083	5	21.798	647275	20.0