LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048984.D
Acq On : 15 Jun 2021 19:23
Operator : CG/JU
Sample : M2672-18
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(76-80)

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: BG048984.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.158	16	20	33	rVB	104827	183082	6.00%	1.240%
2	3.281	37	41	49	rVB	71134	101221	3.32%	0.685%
3	5.191	361	366	374	rBV4	16533	32221	1.06%	0.218%
4	5.667	440	447	454	rBV	727811	1196573	39.20%	8.102%
5	5.731	454	458	469	rVB3	23527	64538	2.11%	0.437%
6	7.271	712	720	730	rBV	728395	1306608	42.81%	8.847%
7	8.117	855	864	870	rBV	124064	220073	7.21%	1.490%
8	9.280	1055	1062	1071	rVB	446579	812769	26.63%	5.503%
9	10.702	1298	1304	1312	rBV2	26696	50140	1.64%	0.340%
10	10.937	1334	1344	1351	rBV	159518	294200	9.64%	1.992%
11	13.381	1753	1760	1767	rBV	1076202	1692069	55.44%	11.457%
12	14.756	1988	1994	2002	rVB	272363	430136	14.09%	2.913%
13	16.155	2227	2232	2238	rBV2	55633	76767	2.52%	0.520%
14	16.243	2240	2247	2261	rVV	1057169	1633738	53.52%	11.063%
15	17.506	2455	2462	2468	rBV	378927	585707	19.19%	3.966%
16	17.623	2476	2482	2486	rBV2	65163	91757	3.01%	0.621%
17	18.164	2570	2574	2579	rVB4	27204	42202	1.38%	0.286%
18	18.387	2607	2612	2623	rBV2	153723	223022	7.31%	1.510%
19	19.656	2823	2828	2838	rBV2	101199	133518	4.37%	0.904%
20	20.115	2900	2906	2912	rVB	2269741	3052299	100.00%	20.668%
21	20.790	3014	3021	3030	rBV	224323	343186	11.24%	2.324%
22	20.873	3032	3035	3038	rVV2	31171	36824	1.21%	0.249%
23	20.914	3038	3042	3047	rVV4	25727	37157	1.22%	0.252%
24	21.431	3125	3130	3136	rBV	141112	224104	7.34%	1.517%
25	21.683	3169	3173	3179	rVB2	57203	84997	2.78%	0.576%
26	21.795	3185	3192	3202	rVB2	386643	676481	22.16%	4.581%
27	22.007	3223	3228	3232	rVB2	28253	42318	1.39%	0.287%
28	22.641	3331	3336	3341	rBV6	26539	51604	1.69%	0.349%
29	23.023	3396	3401	3407	rVB5	36681	69099	2.26%	0.468%
30	23.323	3445	3452	3464	rBV5	93164	258140	8.46%	1.748%
31	25.132	3749	3760	3771	rBV2	224908	688406	22.55%	4.661%
32	26.519	3990	3996	3998	rBV6	17512	33280	1.09%	0.225%

Sum of corrected areas: 14768236

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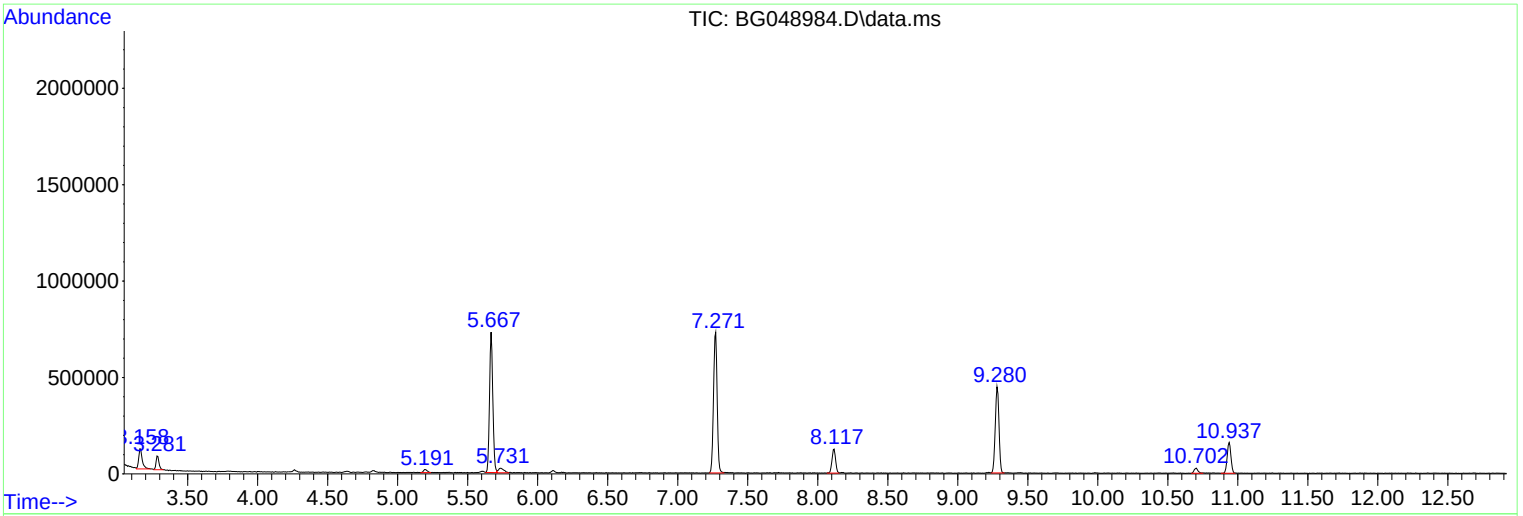
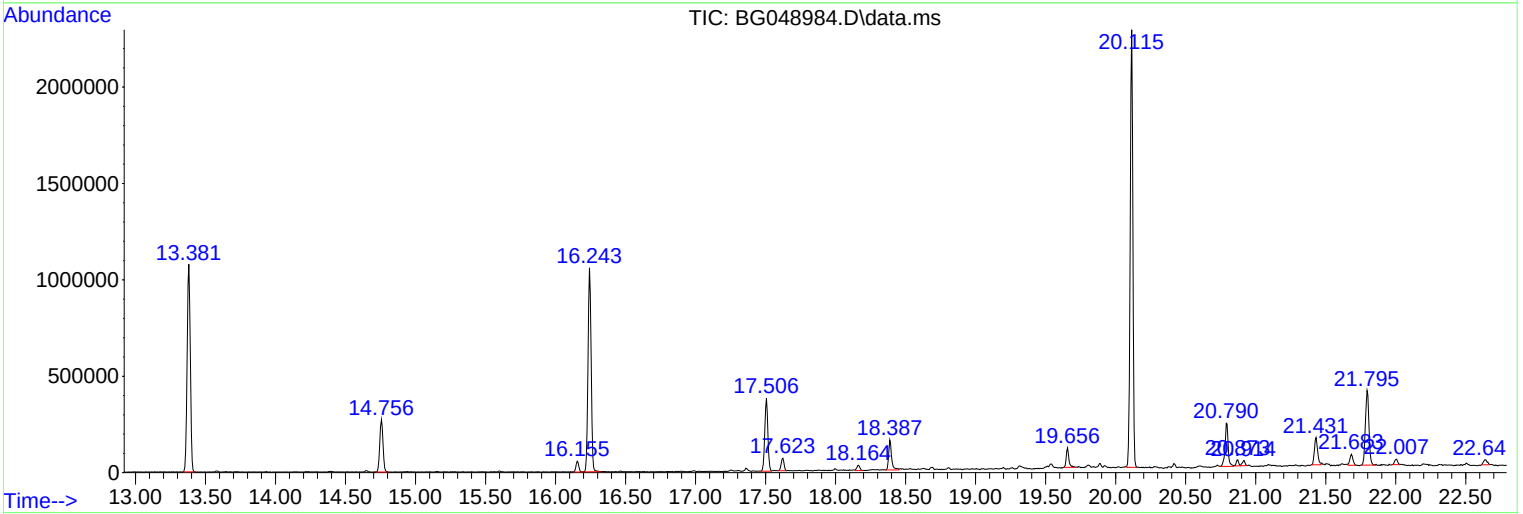
Misc :
ALS Vial : 12 Sample Multiplier: 1

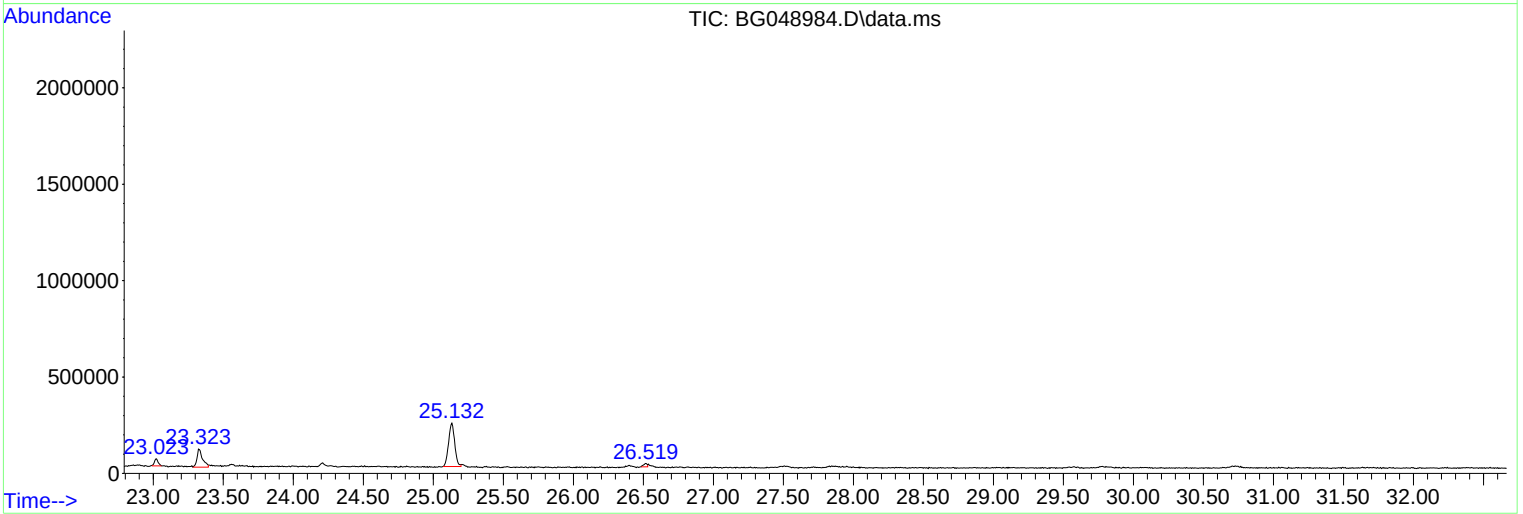
Instrument :
BNA_G
ClientSampleId :
17-B6(76-80)

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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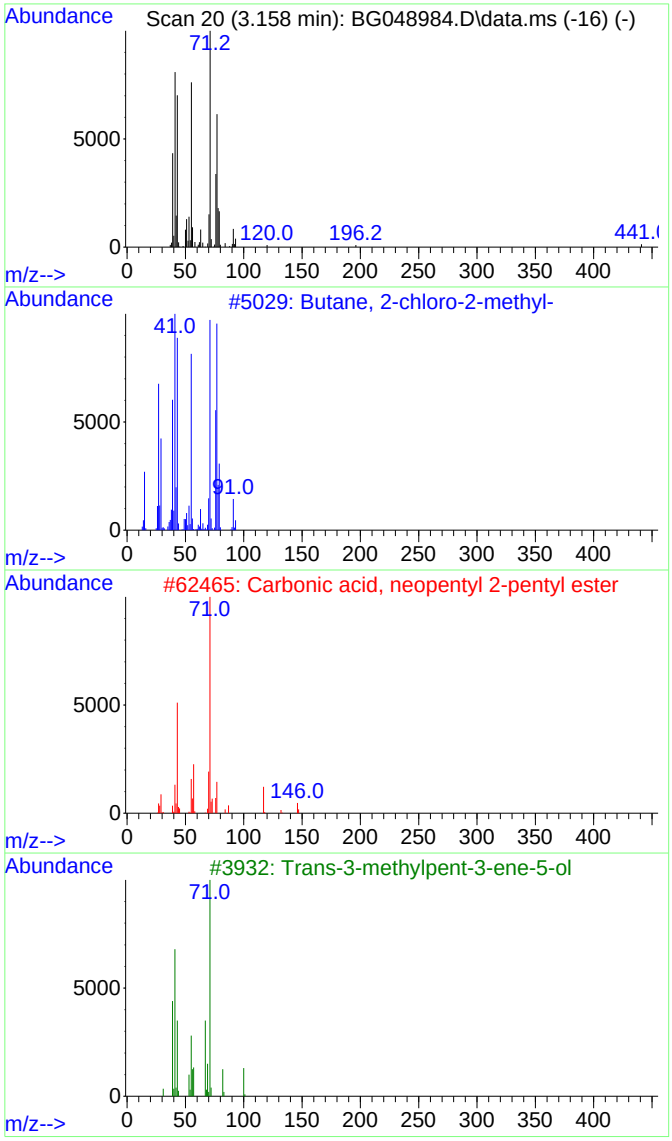
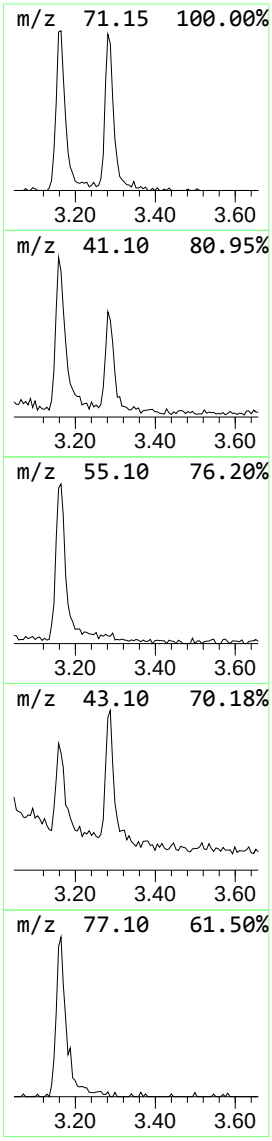
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.158	16.64 ng	183082	1,4-Dichlorobenzene-d4	8.111

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-chloro-2-methyl-	106	C5H11Cl	000594-36-5	83
2	Carbonic acid, neopentyl 2-penty...	202	C11H22O3	1000357-85-4	25
3	Trans-3-methylpent-3-ene-5-ol	100	C6H12O	030801-95-7	25
4	1-Hexene, 4,5-dimethyl-	112	C8H16	016106-59-5	25
5	2-[Dimethyl(pentafluorophenyl)si...	326	C13H15F5O2Si	1000216-80-8	23





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Data File : BG048984.D
Acq On : 15 Jun 2021 19:23
Operator : CG/JU
Sample : M2672-18
Misc :
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Instrument : BNA_G
ClientSampleId : 17-B6(76-80)

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

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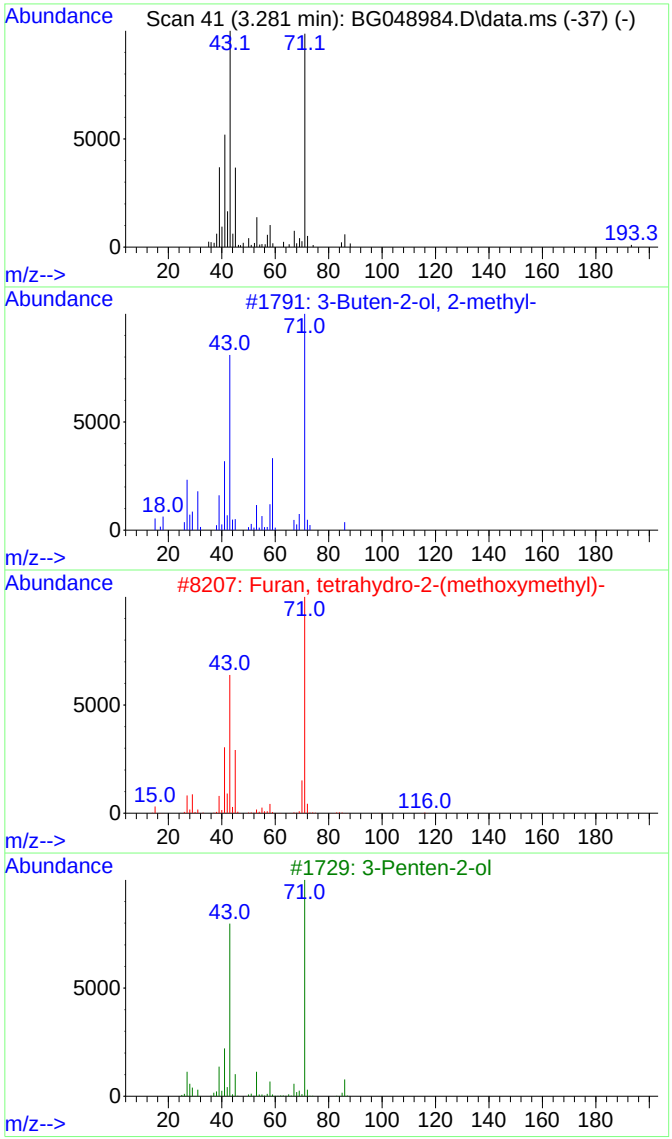
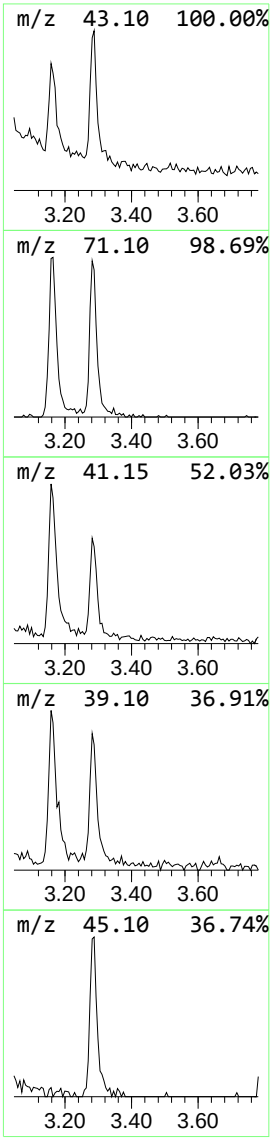
****
Peak Number 2 3-Buten-2-ol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.281	9.20 ng	101221	1,4-Dichlorobenzene-d4	8.111

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	80
2	Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	72
3	3-Penten-2-ol	86	C5H10O	001569-50-2	64
4	Acetic acid, (1,2-dimethyl-1-pro...	128	C7H12O2	003814-41-3	64
5	Pentane, 2,2'-oxybis-	158	C10H22O	056762-00-6	64





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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
17-B6(76-80)

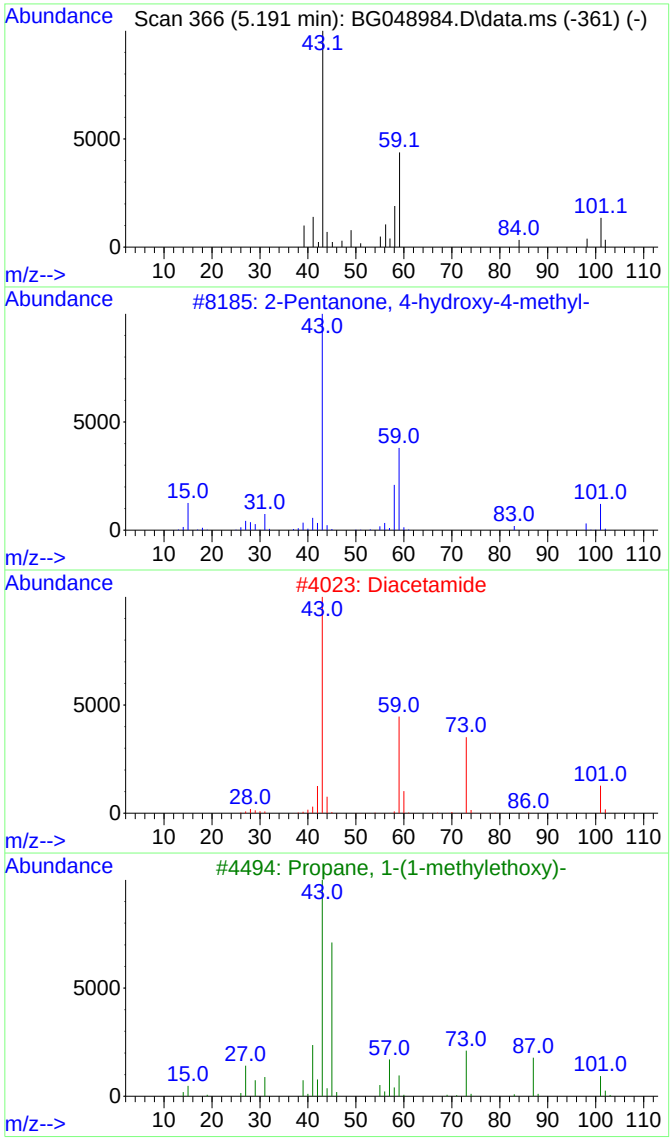
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

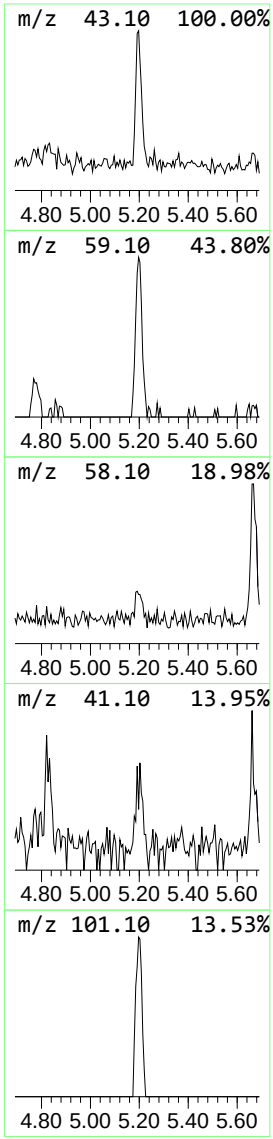
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.191	2.93 ng	32221	1,4-Dichlorobenzene-d4	8.111

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Diacetamide	101	C4H7NO2	000625-77-4	33
3	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	9
4	Formamide, N-butyl-	101	C5H11NO	000871-71-6	9
5	2-Propanone, 1-cyclopropyl-	98	C6H10O	004160-75-2	9





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17-B6(76-80)

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

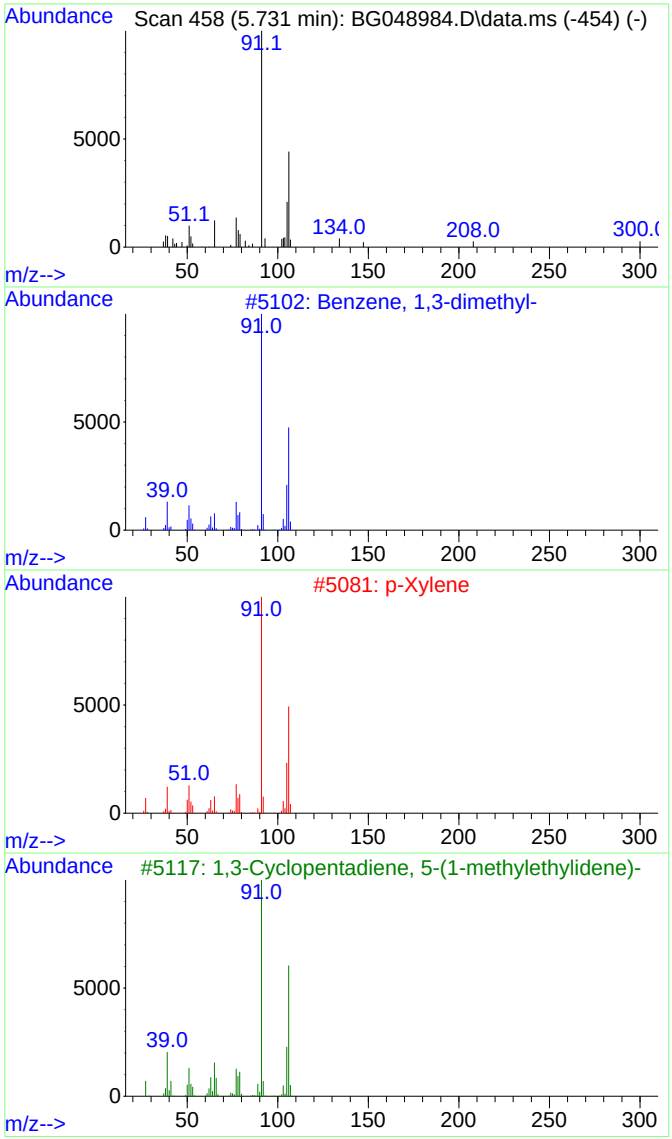
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

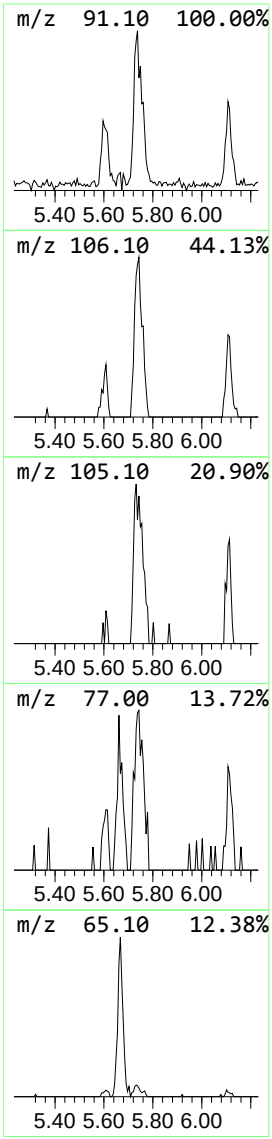
****

Peak Number 4 Benzene, 1,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.731	5.87 ng	64538	1,4-Dichlorobenzene-d4	8.111

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	1,3-Cyclopentadiene, 5-(1-methyl...	106	C8H10	002175-91-9	72
4	o-Xylene	106	C8H10	000095-47-6	64
5	Cyclopentene, 1-ethenyl-3-methyl...	106	C8H10	061142-07-2	59





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Instrument :
BNA_G
ClientSampleId :
17-B6(76-80)

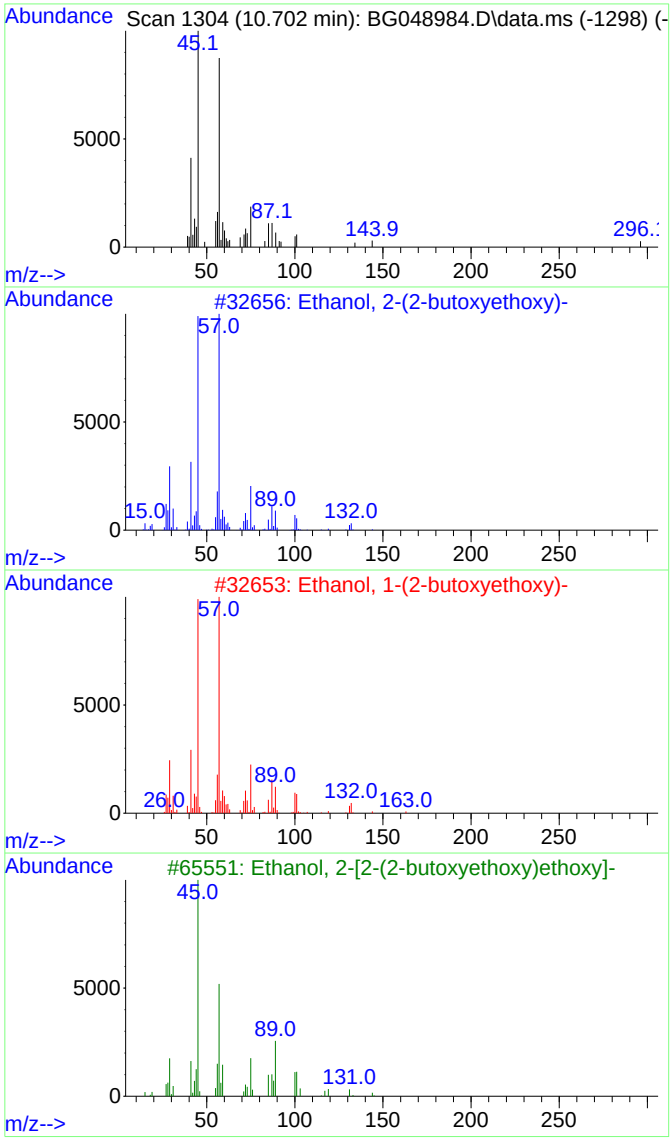
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

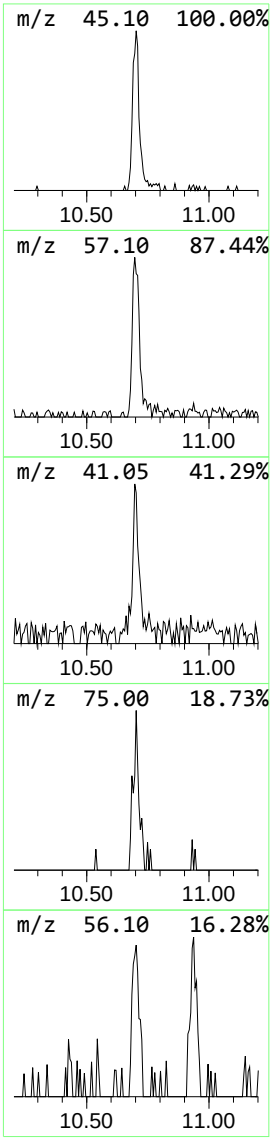
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.702	3.41 ng	50140	Naphthalene-d8	10.937

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	78
3	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	50
4	2-Hexanol, 5-methyl-	116	C7H16O	000627-59-8	43
5	3,6,9,12-Tetraoxahexadecan-1-ol	250	C12H26O5	001559-34-8	42





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Instrument :
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17-B6(76-80)

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

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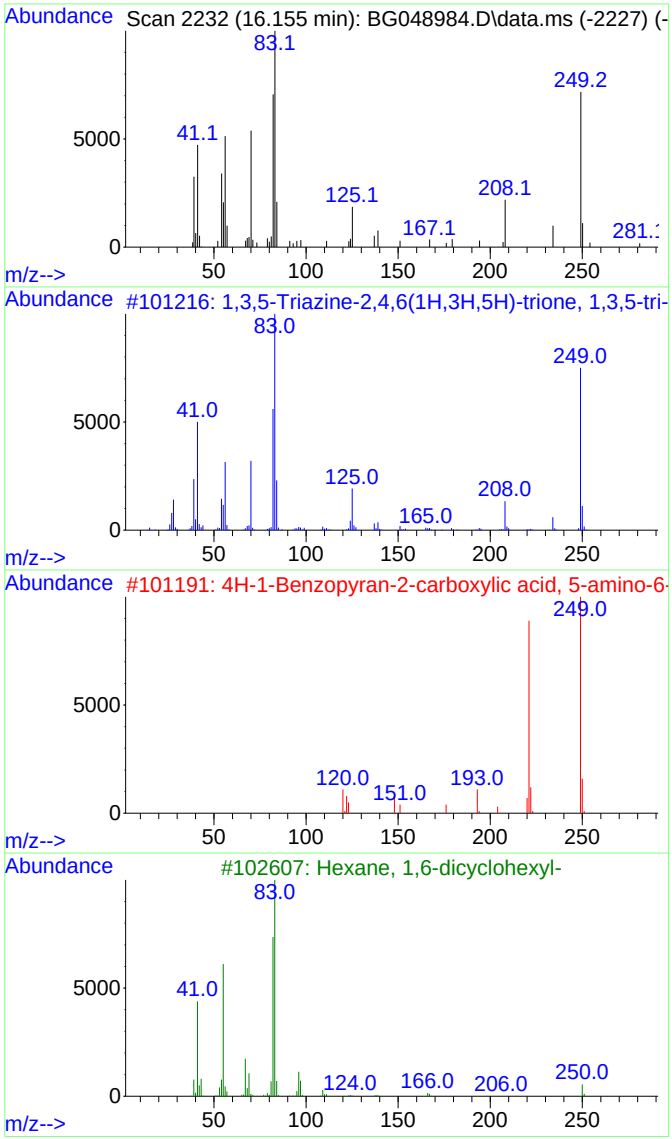
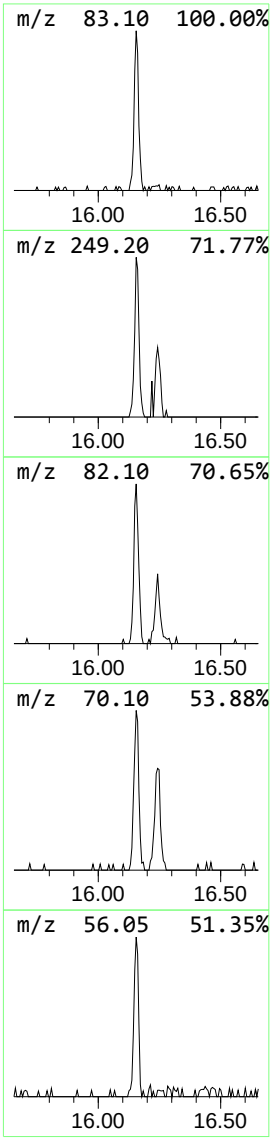
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1,3,5-Triazine-2,4,6(1H,3H,... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.155	2.62 ng	76767	Phenanthrene-d10	17.506

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	93
2	4H-1-Benzopyran-2-carboxylic aci...	249	C12H11NO5	032142-43-1	37
3	Hexane, 1,6-dicyclohexyl-	250	C18H34	001610-23-7	35
4	Cyclohexane, undecyl-	238	C17H34	054105-66-7	16
5	Cyclohexane, octyl-	196	C14H28	001795-15-9	12





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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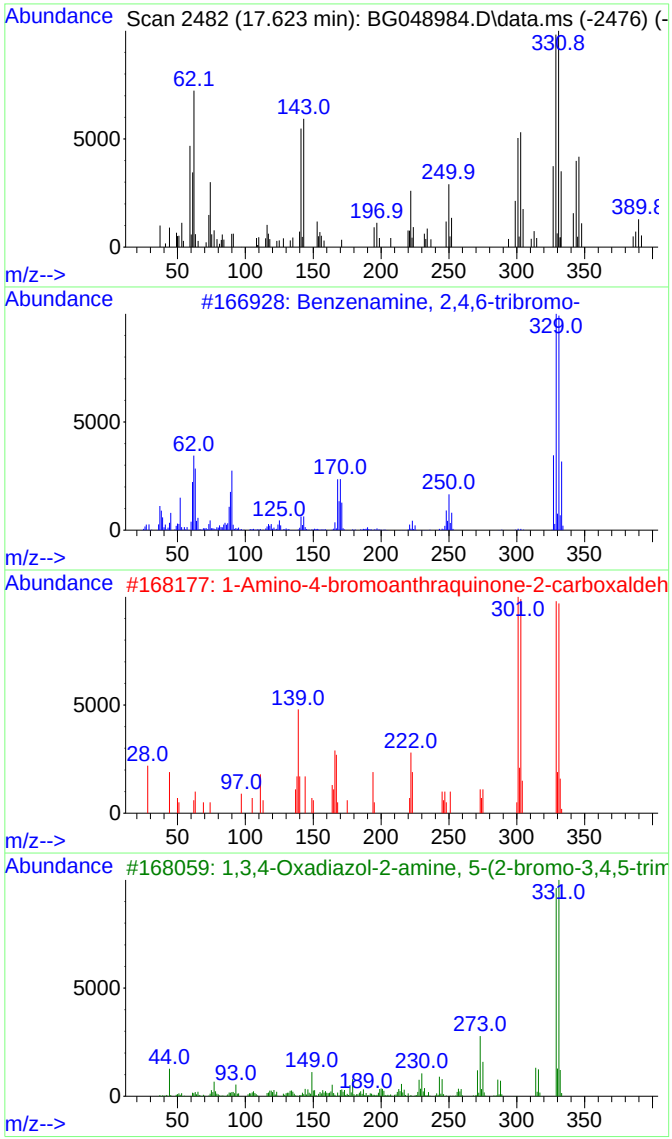
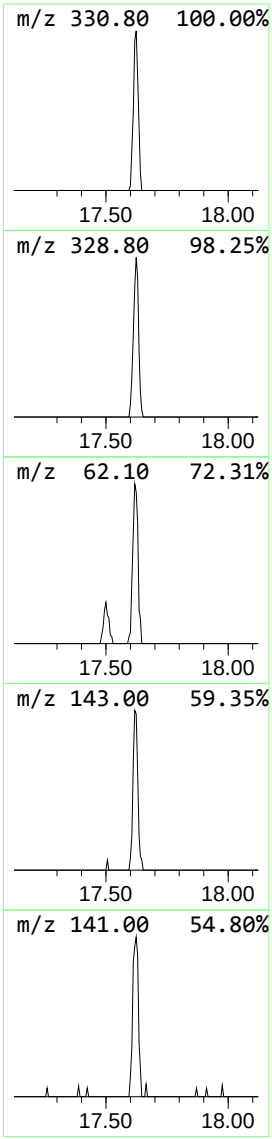
****

Peak Number 7 Benzenamine, 2,4,6-tribromo- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.624	3.13 ng	91757	Phenanthrene-d10	17.506

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenamine, 2,4,6-tribromo-	327	C6H4Br3N	000147-82-0	50
2	1-Amino-4-bromoanthraquinone-2-c...	329	C15H8BrNO3	062823-21-6	25
3	1,3,4-Oxadiazol-2-amine, 5-(2-br...	329	C11H12BrN3O4	1000350-74-8	14
4	Bromophos	364	C8H8BrCl2O3PS	002104-96-3	12
5	4,4'-(p-Phenylenediisopropyliden...	344	C24H28N2	002716-10-1	10





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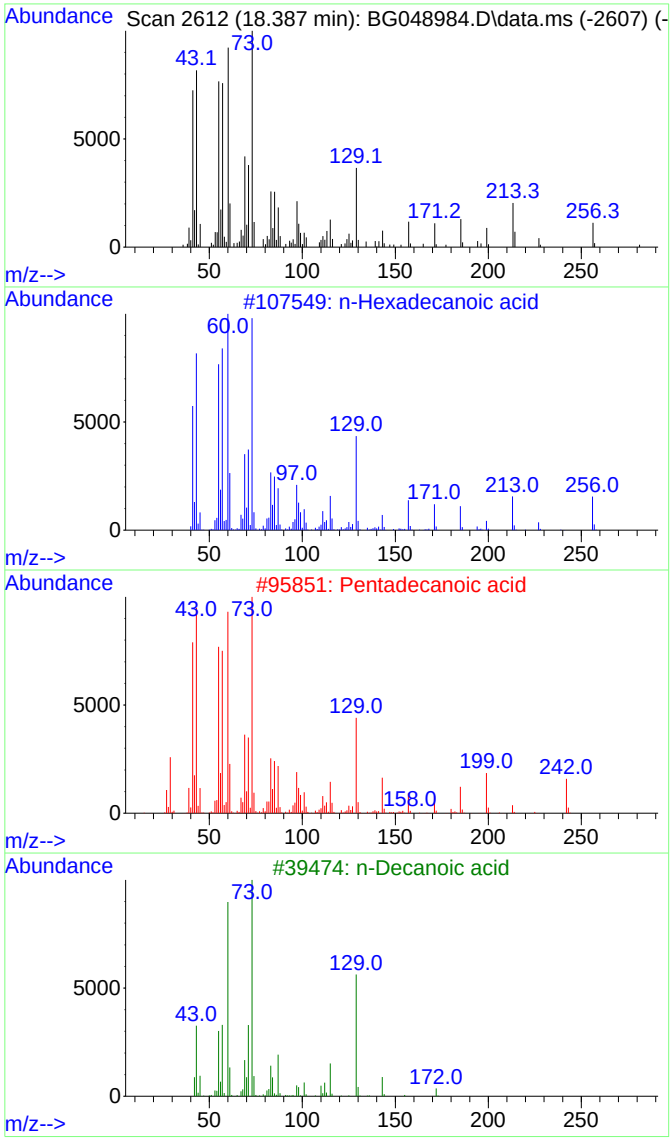
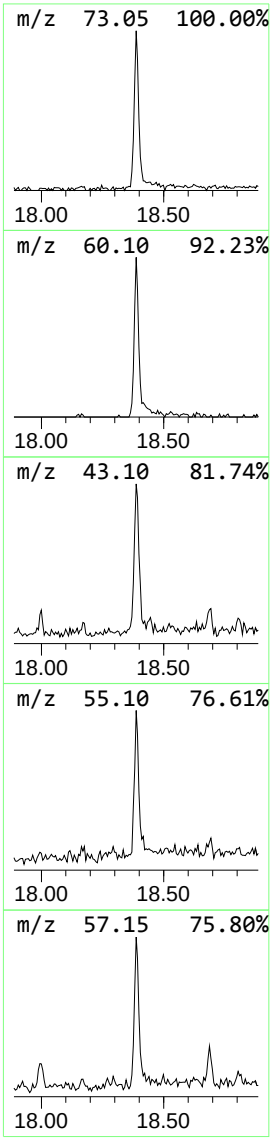
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.387	7.62 ng	223022	Phenanthrene-d10	17.506

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3	n-Decanoic acid	172	C10H20O2	000334-48-5	78
4	Undecanoic acid	186	C11H22O2	000112-37-8	76
5	Tridecanoic acid	214	C13H26O2	000638-53-9	74





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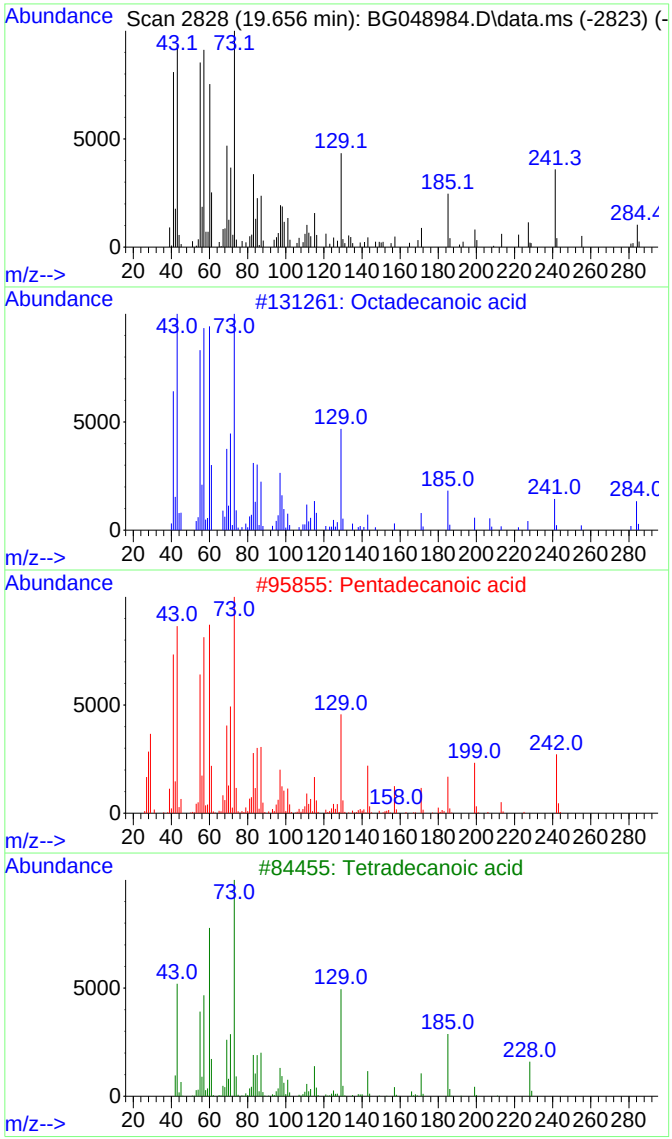
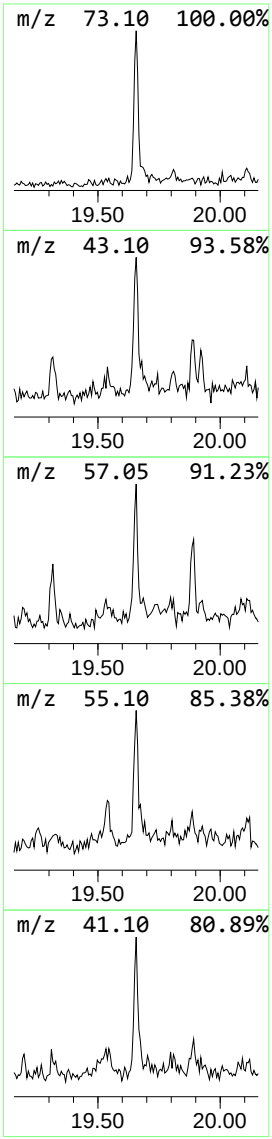
****

Peak Number 9 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.656	3.95 ng	133518	Chrysene-d12	21.795

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048984.D
Acq On : 15 Jun 2021 19:23
Operator : CG/JU
Sample : M2672-18
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(76-80)

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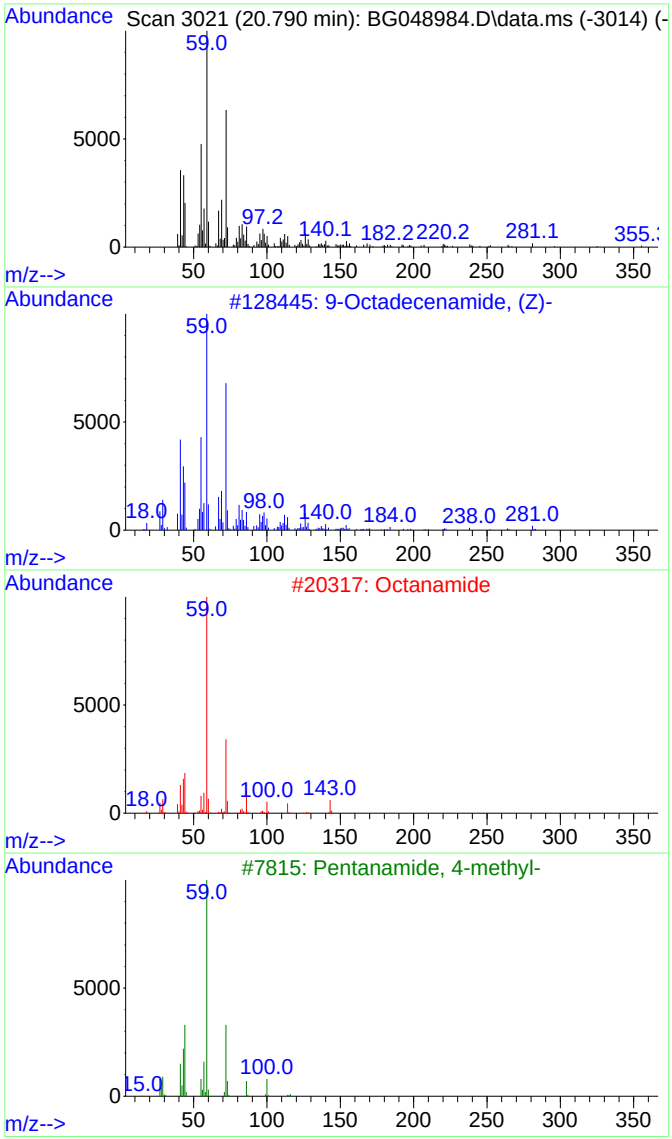
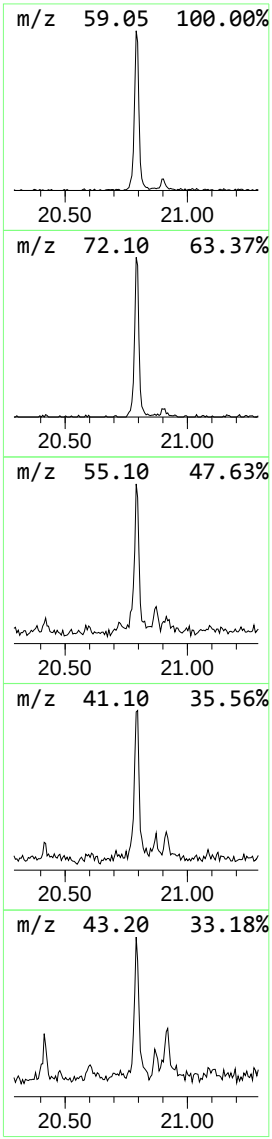
Peak Number 10 9-Octadecenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.790	10.15 ng	343186	Chrysene-d12	21.795

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	99
2	Octanamide	143	C8H17NO	000629-01-6	72
3	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	59
4	Tetradecanamide	227	C14H29NO	000638-58-4	56
5	Hexadecanamide	255	C16H33NO	000629-54-9	53





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Data File : BG048984.D
Acq On : 15 Jun 2021 19:23
Operator : CG/JU
Sample : M2672-18
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(76-80)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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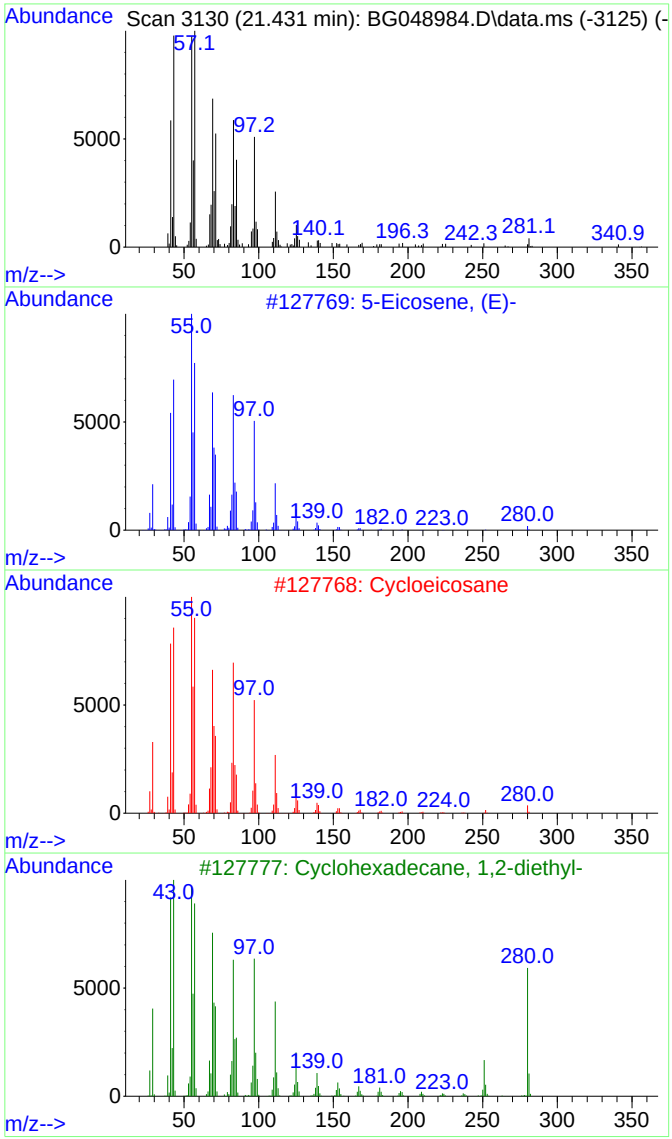
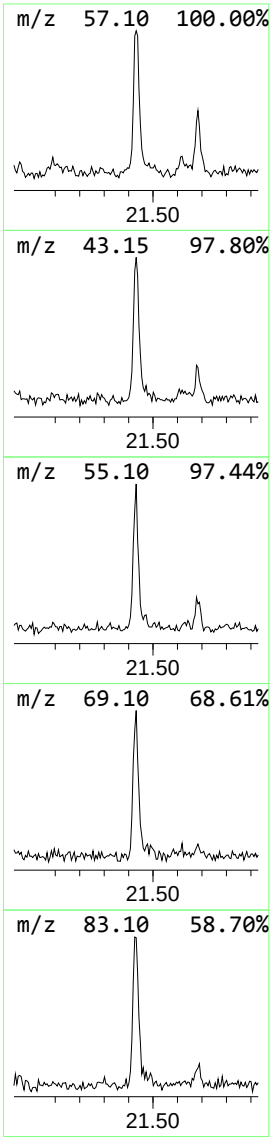
Peak Number 11 5-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.431	6.63 ng	224104	Chrysene-d12	21.795

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	96
2	Cycloeicosane	280	C20H40	000296-56-0	96
3	Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	93
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	92
5	9-Eicosene, (E)-	280	C20H40	074685-29-3	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048984.D
Acq On : 15 Jun 2021 19:23
Operator : CG/JU
Sample : M2672-18
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(76-80)

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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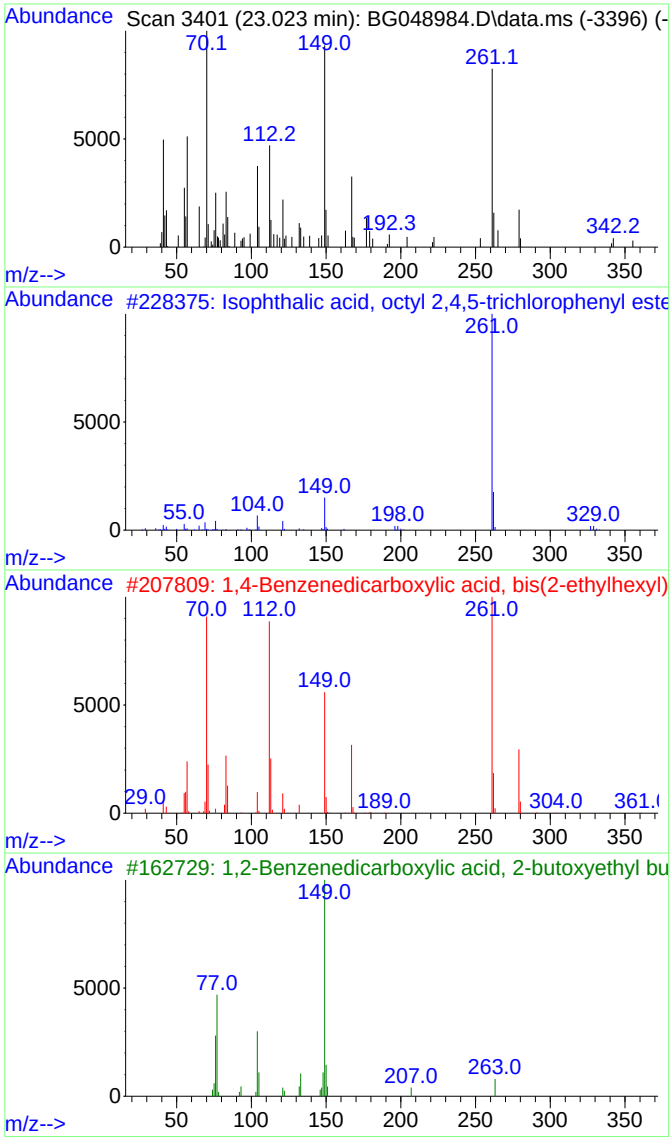
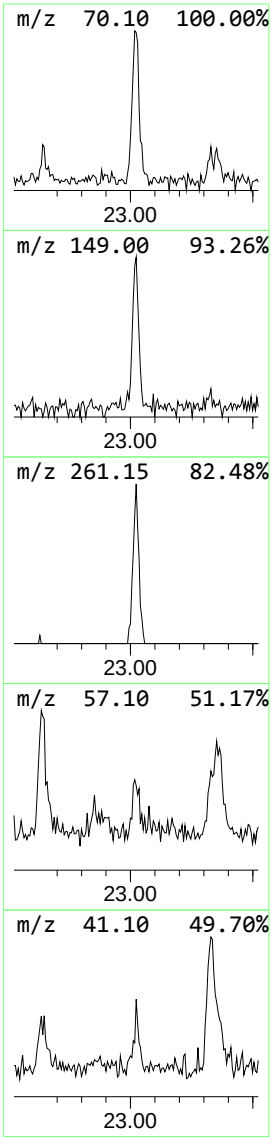
Peak Number 12 unknown23.023 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.023	2.04 ng	69099	Chrysene-d12	21.795

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isophthalic acid, octyl 2,4,5-tr...	456	C22H23Cl3O4	1000356-61-5	43
2	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	35
3	1,2-Benzenedicarboxylic acid, 2-...	322	C18H26O5	033374-28-6	27
4	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	22
5	Diisooctyl phthalate	390	C24H38O4	000131-20-4	22





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Acq On : 15 Jun 2021 19:23
Operator : CG/JU
Sample : M2672-18
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
17-B6(76-80)

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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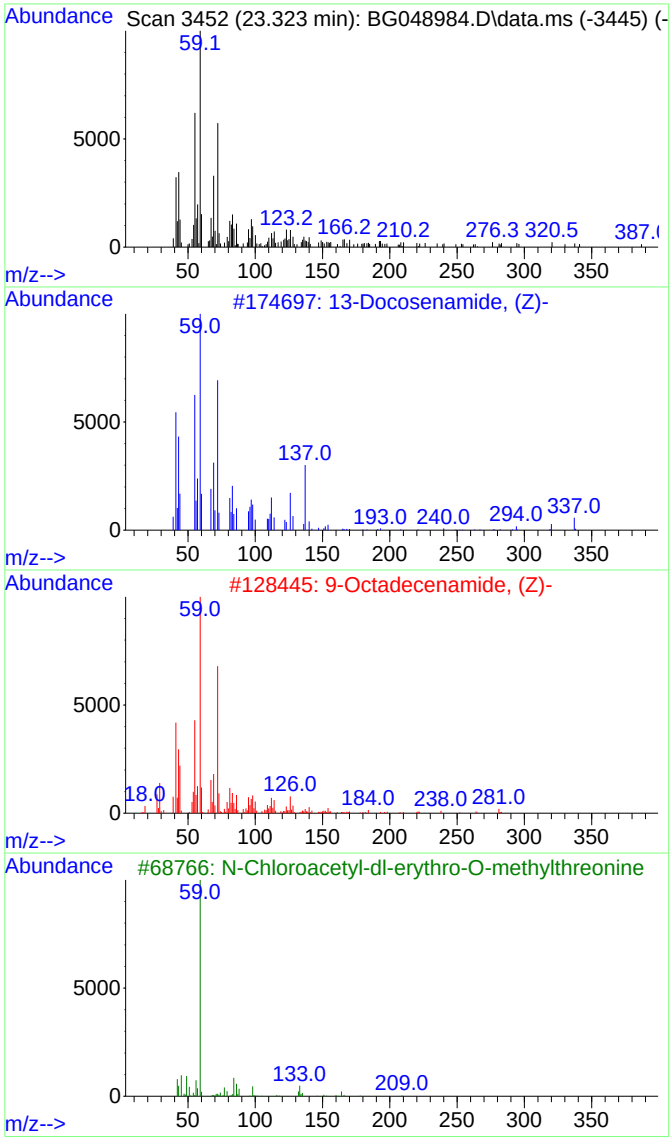
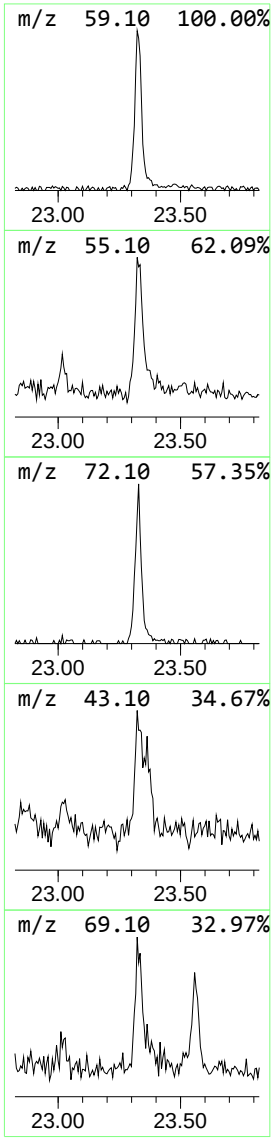
Peak Number 13 13-Docosenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.323	7.63 ng	258140	Chrysene-d12	21.795

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	91
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
3	N-Chloroacetyl-dl-erythro-O-meth...	209	C7H12ClNO4	1000214-48-1	43
4	2,7-Dioxatricyclo[4.4.0.0(3,8)]d...	155	C8H13NO2	040076-28-6	11
5	N-(3-Methylbutyl)acetamide	129	C7H15NO	013434-12-3	11





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048984.D
Acq On : 15 Jun 2021 19:23
Operator : CG/JU
Sample : M2672-18
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(76-80)

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...	3.158	16.6	ng	183082	1	8.111	220073	20.0
3-Buten-2-ol, 2...	3.281	9.2	ng	101221	1	8.111	220073	20.0
2-Pentanone, 4-...	5.191	2.9	ng	32221	1	8.111	220073	20.0
Benzene, 1,3-di...	5.731	5.9	ng	64538	1	8.111	220073	20.0
Ethanol, 2-(2-b...	10.702	3.4	ng	50140	2	10.937	294200	20.0
1,3,5-Triazine-...	16.155	2.6	ng	76767	4	17.506	585707	20.0
Benzenamine, 2,...	17.624	3.1	ng	91757	4	17.506	585707	20.0
n-Hexadecanoic ...	18.387	7.6	ng	223022	4	17.506	585707	20.0
Octadecanoic acid	19.656	4.0	ng	133518	5	21.795	676481	20.0
9-Octadecenamid...	20.790	10.2	ng	343186	5	21.795	676481	20.0
5-Eicosene, (E)-	21.431	6.6	ng	224104	5	21.795	676481	20.0
unknown23.023	23.023	2.0	ng	69099	5	21.795	676481	20.0
13-Docosenamide...	23.323	7.6	ng	258140	5	21.795	676481	20.0