LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081122\
Data File : BG054600.D
Acq On : 11 Aug 2022 11:42
Operator : CG/JU
Sample : N3971-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-20R

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-BG071522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054600.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.089	11	17	34	rVB	229970	392221	23.71%	6.108%
2	4.405	234	241	256	rVB	52487	90917	5.50%	1.416%
3	5.051	344	351	361	rBV2	15670	26501	1.60%	0.413%
4	5.557	431	437	450	rVB	101577	183036	11.06%	2.851%
5	6.602	609	615	623	rBB2	14207	22887	1.38%	0.356%
6	7.178	707	713	726	rVB	62766	116700	7.05%	1.817%
7	7.971	841	848	854	rBV	47530	80626	4.87%	1.256%
8	8.030	854	858	873	rVB	13343	27348	1.65%	0.426%
9	9.135	1039	1046	1056	rBV	138404	260116	15.72%	4.051%
10	10.780	1319	1326	1332	rBV	60836	109387	6.61%	1.704%
11	11.720	1481	1486	1499	rVB3	13458	32244	1.95%	0.502%
12	13.230	1734	1743	1750	rBV	452204	718103	43.40%	11.184%
13	13.465	1776	1783	1792	rBV	139754	227011	13.72%	3.535%
14	14.611	1972	1978	1985	rBV	114957	181727	10.98%	2.830%
15	16.109	2227	2233	2247	rBV	439960	704432	42.58%	10.971%
16	17.360	2439	2446	2453	rBV	165161	257990	15.59%	4.018%
17	18.013	2551	2557	2561	rBV2	20182	24349	1.47%	0.379%
18	18.253	2589	2598	2611	rBV4	17905	55200	3.34%	0.860%
19	19.452	2793	2802	2809	rBV2	27278	67516	4.08%	1.051%
20	19.969	2883	2890	2896	rBV	1257600	1654459	100.00%	25.766%
21	20.345	2948	2954	2961	rBV2	41310	83998	5.08%	1.308%
22	21.127	3081	3087	3094	rVB	42283	77208	4.67%	1.202%
23	21.626	3165	3172	3179	rBV	232143	378059	22.85%	5.888%
24	21.973	3225	3231	3241	rVB3	34178	82244	4.97%	1.281%
25	22.966	3393	3400	3407	rVB5	25276	63052	3.81%	0.982%
26	24.117	3590	3596	3607	rVB5	22969	64726	3.91%	1.008%
27	24.828	3708	3717	3731	rVB	133456	393187	23.77%	6.123%
28	25.480	3823	3828	3838	rVB7	14564	45738	2.76%	0.712%

Sum of corrected areas: 6420982

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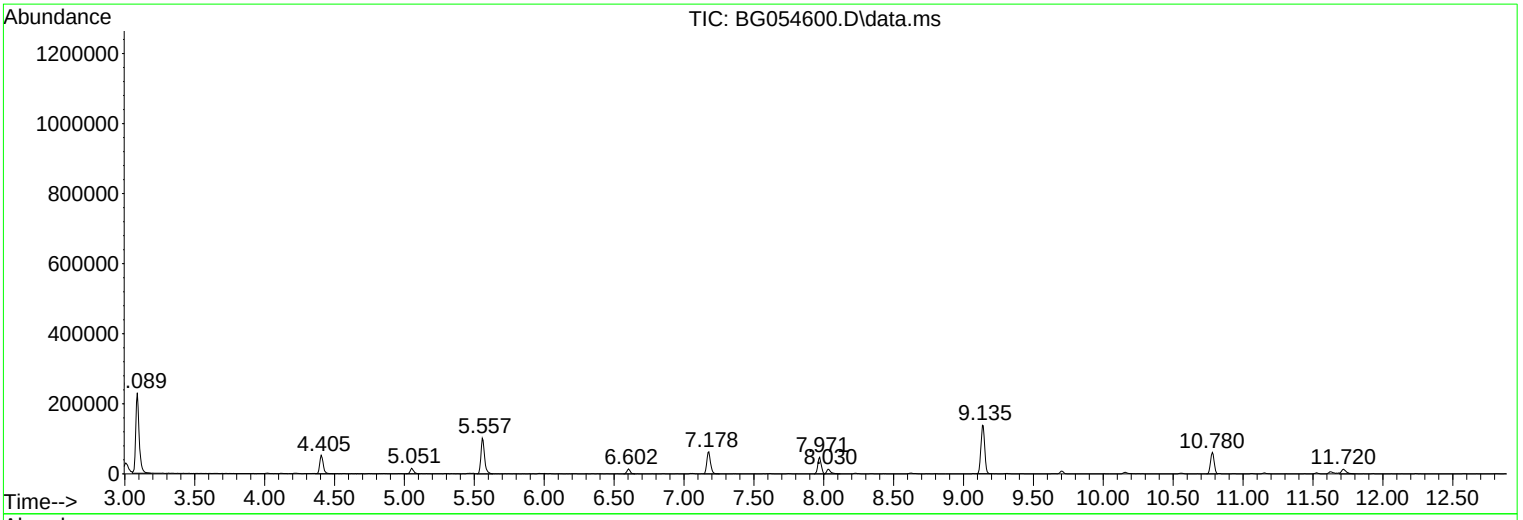
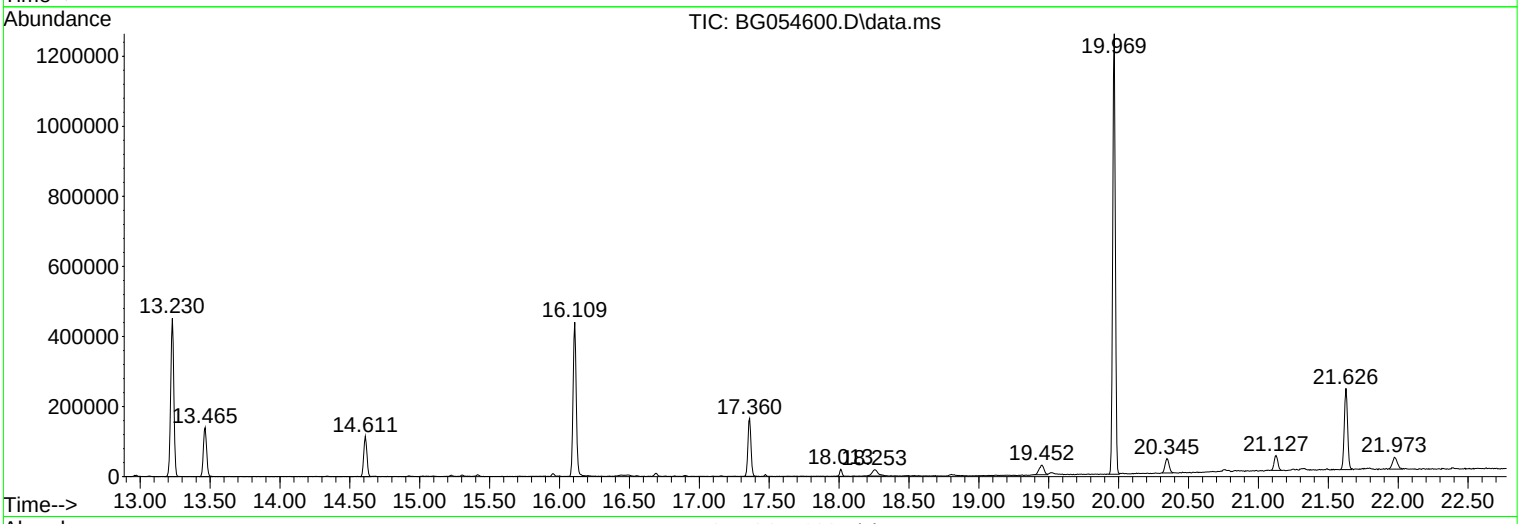
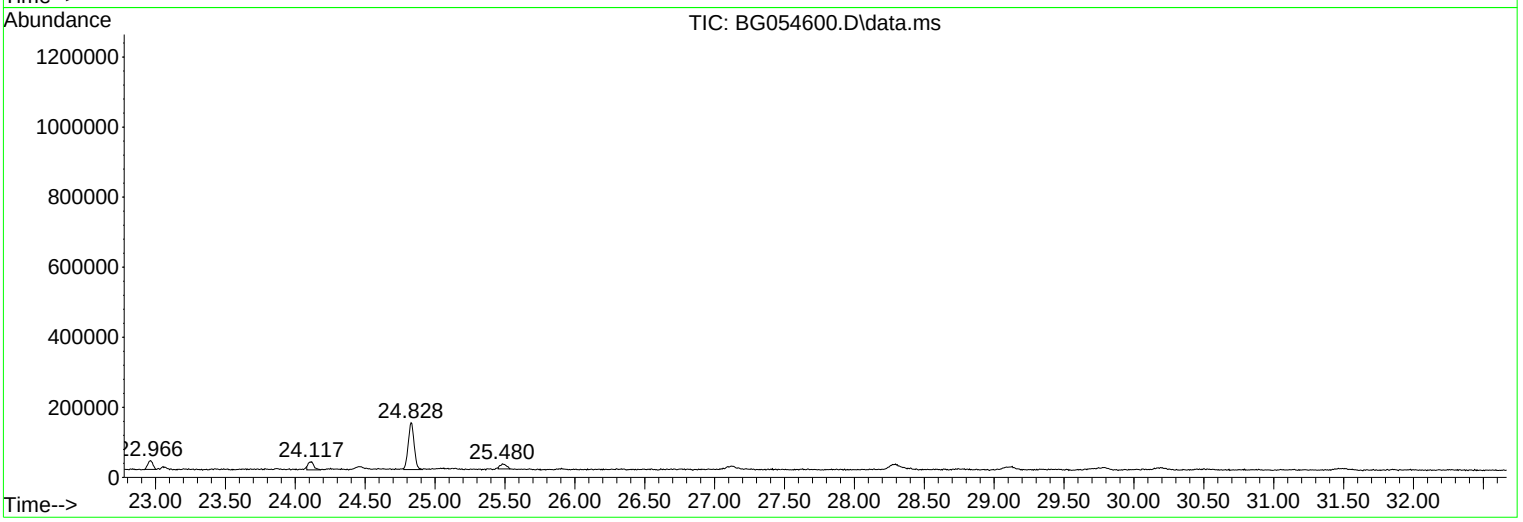
MW-20R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







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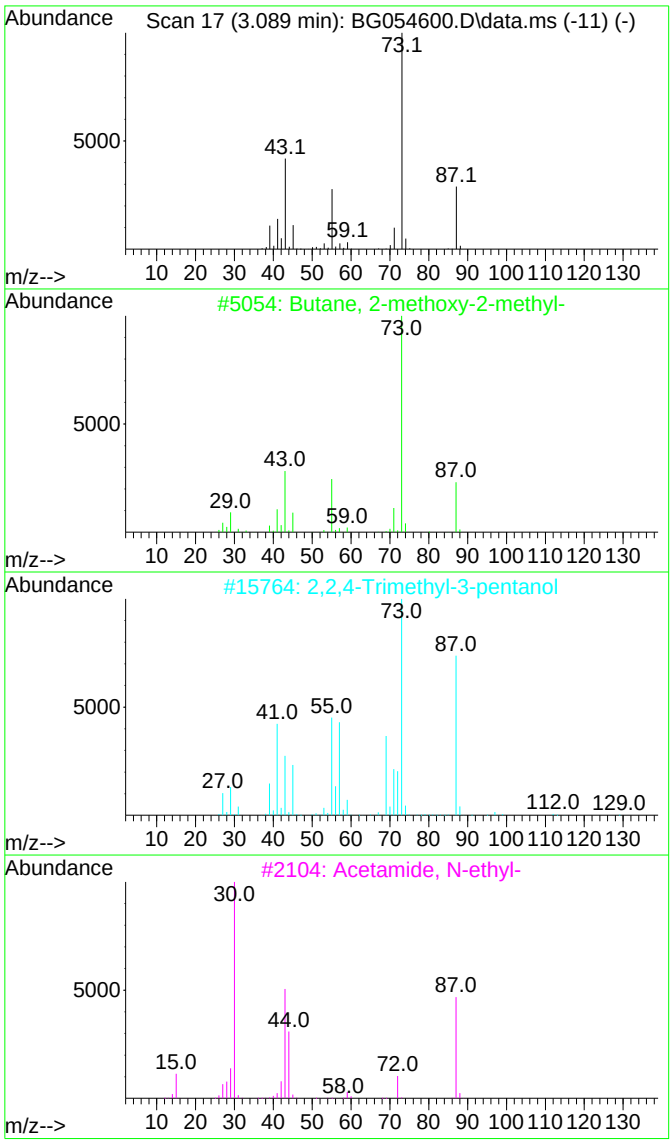
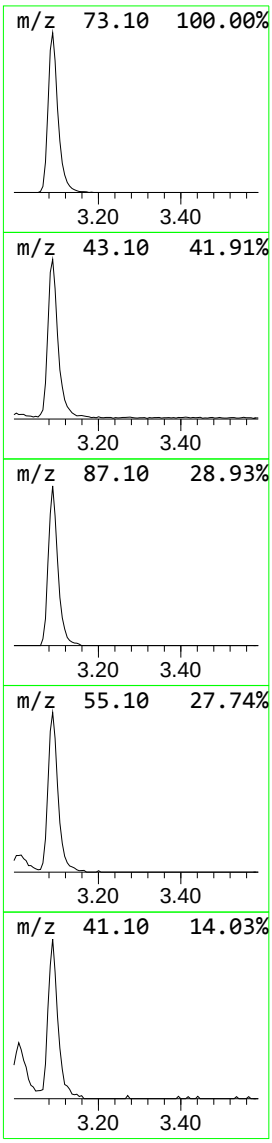
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.089	97.29 ng	392221	1,4-Dichlorobenzene-d4	7.971

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	35
4	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Operator : CG/JU
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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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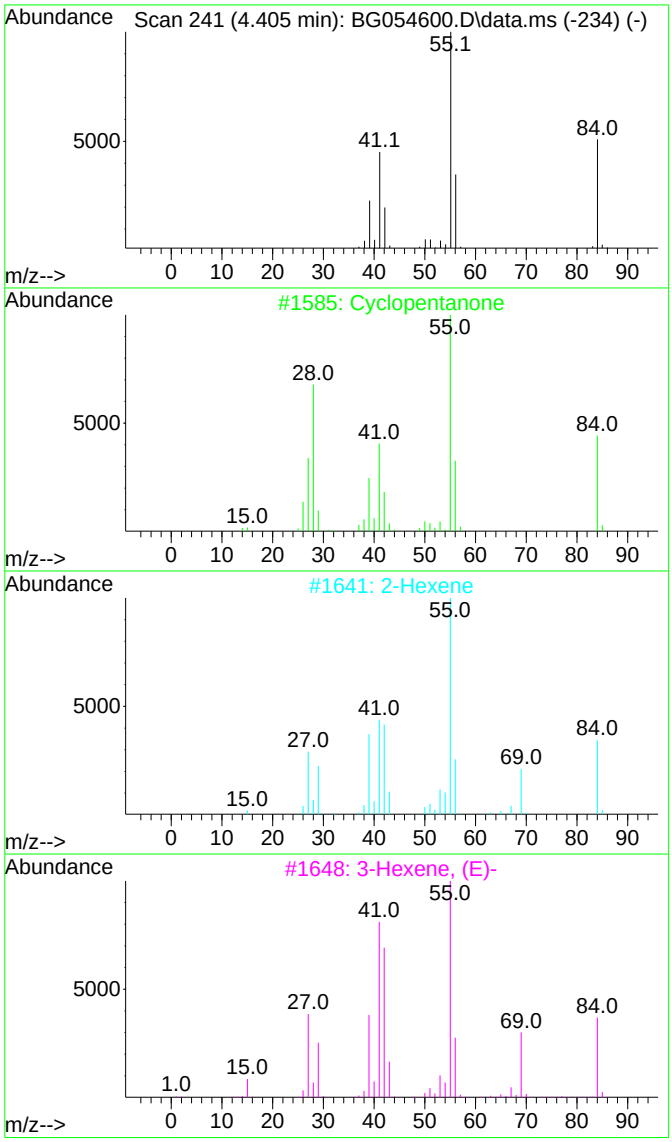
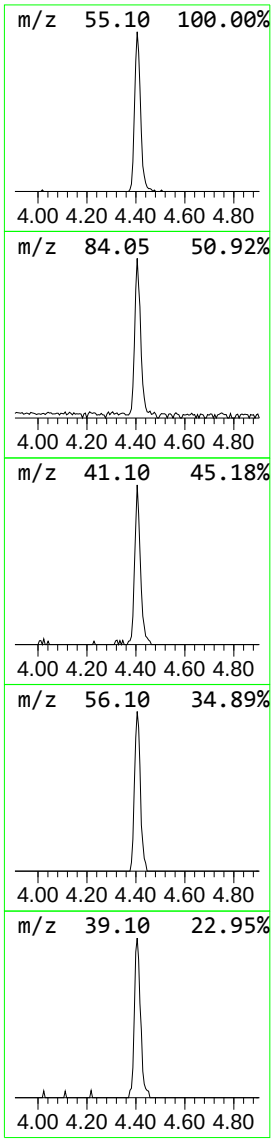
Peak Number 2 Cyclopentanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.405	22.55 ng	90917	1,4-Dichlorobenzene-d4	7.971

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanone	84	C5H8O	000120-92-3	91
2	2-Hexene	84	C6H12	000592-43-8	64
3	3-Hexene, (E)-	84	C6H12	013269-52-8	53
4	2H-Pyran, 3,4-dihydro-	84	C5H8O	000110-87-2	53
5	2-Amino-oxazole	84	C3H4N2O	004570-45-0	50





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Sample : N3971-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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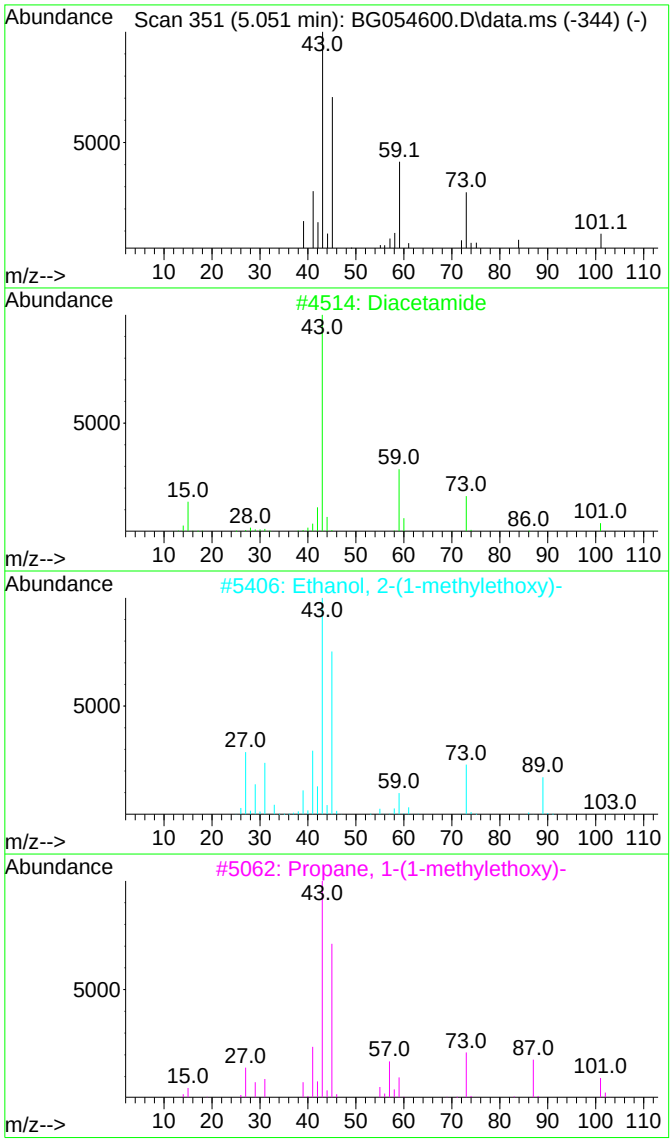
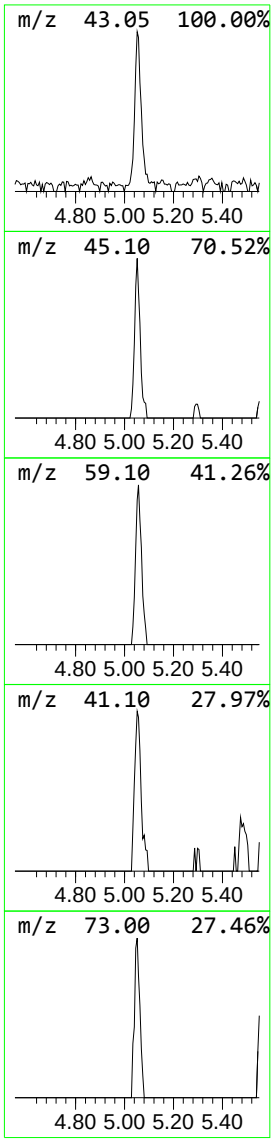
Peak Number 3 unknown5.051 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.051	6.57 ng	26501	1,4-Dichlorobenzene-d4	7.971

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diacetamide	101	C4H7NO2	000625-77-4	43
2	Ethanol, 2-(1-methylethoxy)-	104	C5H12O2	000109-59-1	38
3	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	33
4	2-Propanol, 1-propoxy-	118	C6H14O2	001569-01-3	28
5	Ethanol, 2-propoxy-	104	C5H12O2	002807-30-9	25





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Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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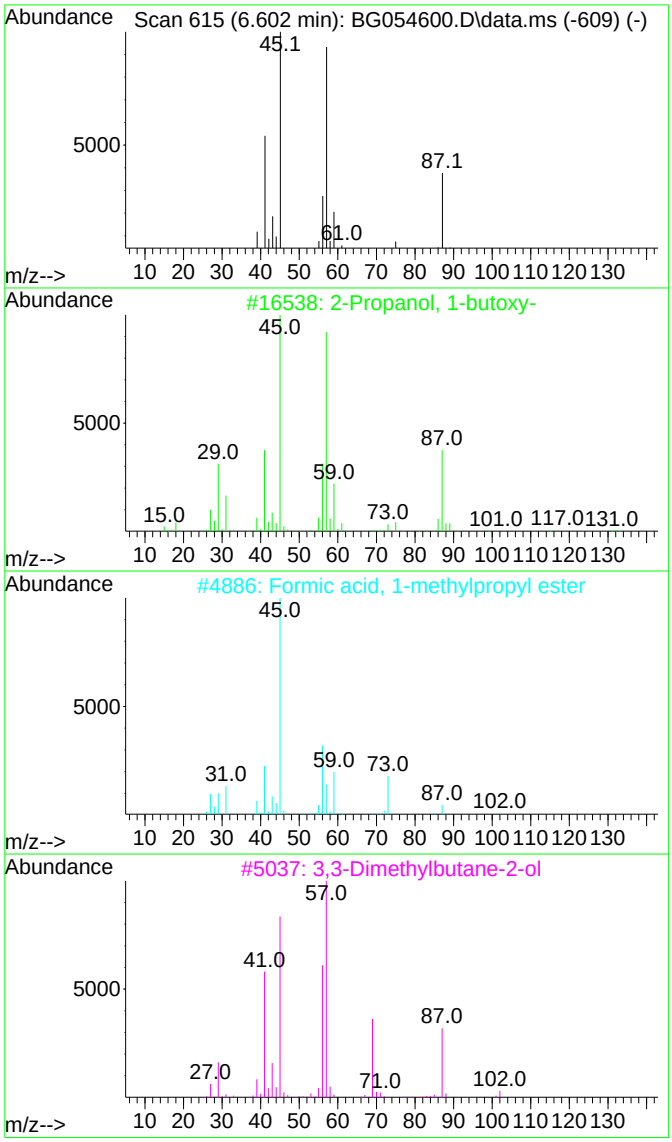
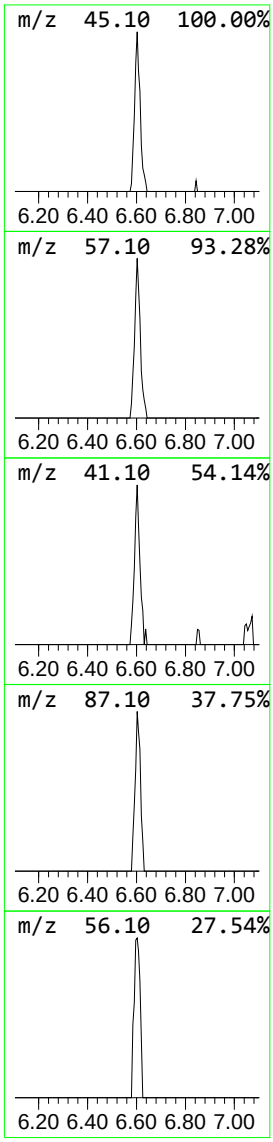
Peak Number 4 2-Propanol, 1-butoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.602	5.68 ng	22887	1,4-Dichlorobenzene-d4	7.971

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	83
2	Formic acid, 1-methylpropyl ester	102	C5H10O2	000589-40-2	38
3	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	33
4	Morpholine	87	C4H9NO	000110-91-8	14
5	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9





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ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
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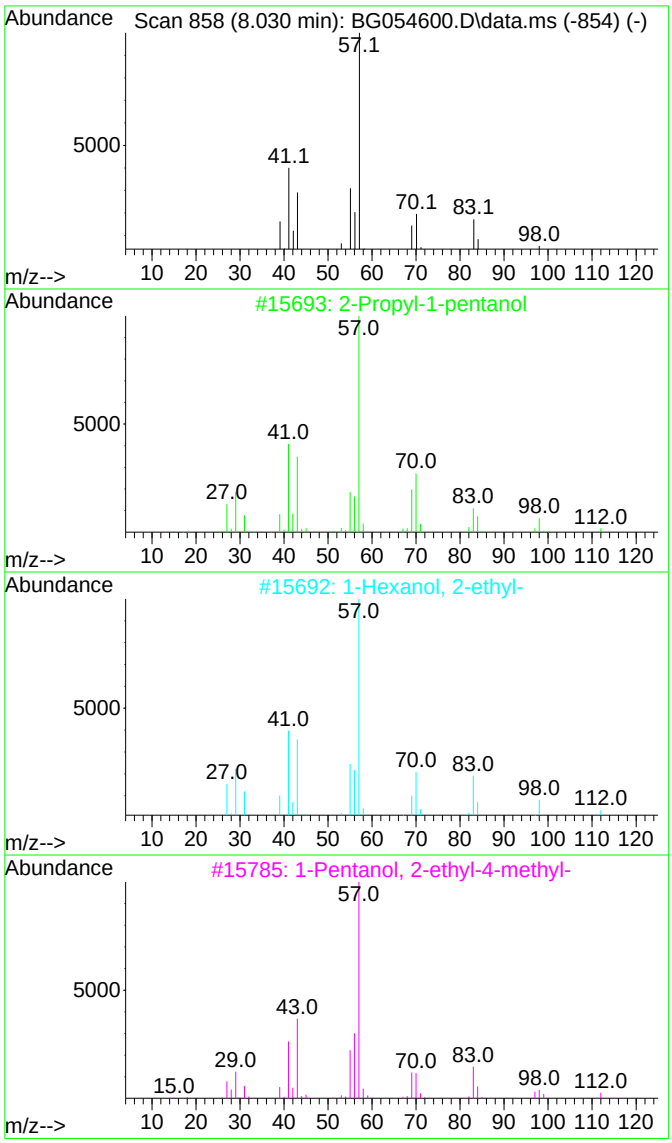
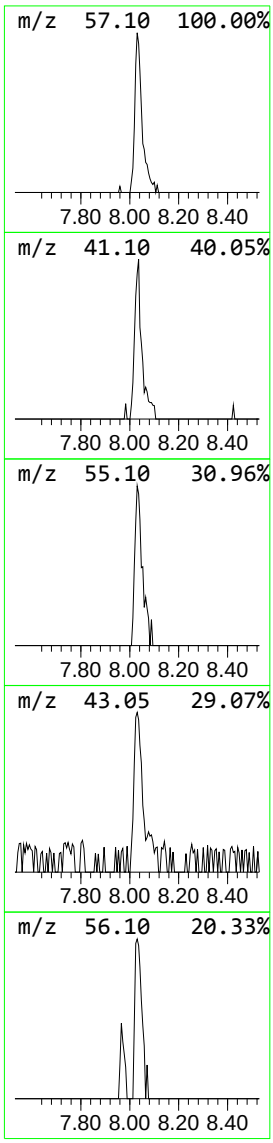
Peak Number 5 2-Propyl-1-pentanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.030	6.78 ng	27348	1,4-Dichlorobenzene-d4	7.971

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	78
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
3	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	50
4	1-Octyn-3-ol, 4-ethyl-	154	C10H18O	005877-42-9	40
5	Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	36





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
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TIC Library : C:\Database\NIST20.L
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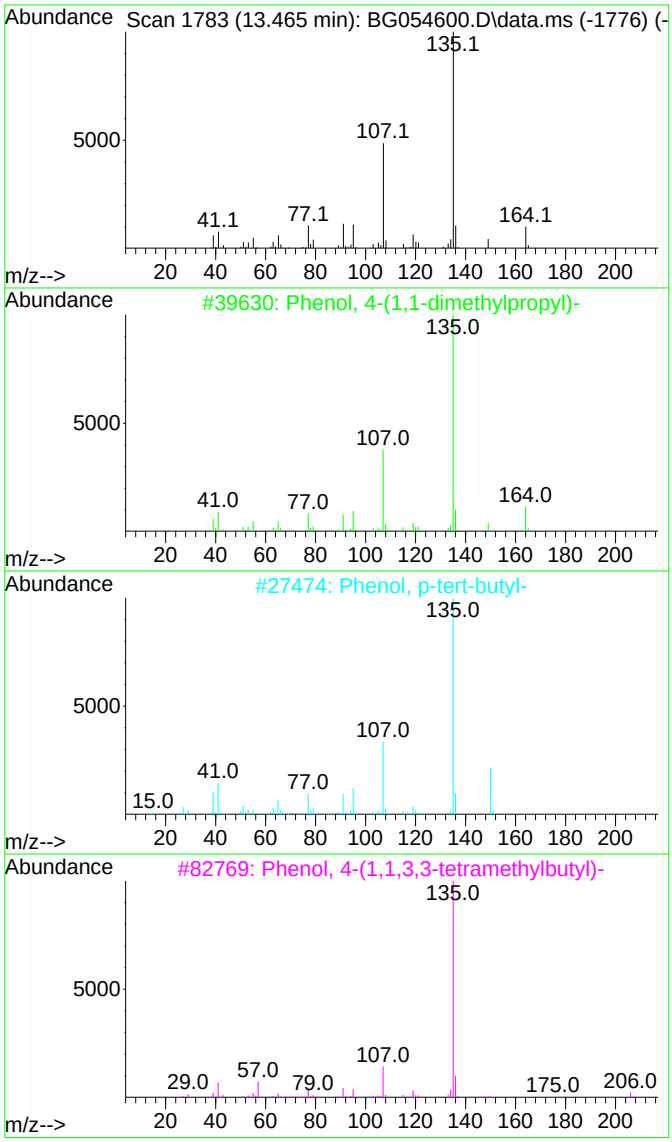
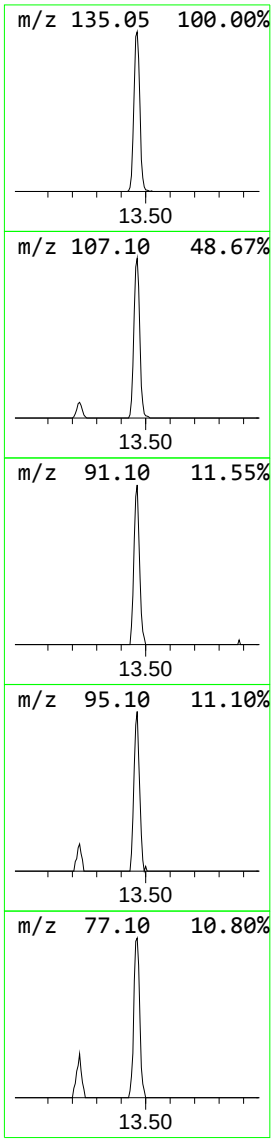
Peak Number 6 Phenol, 4-(1,1-dimethylprop... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.465	24.98 ng	227011	Acenaphthene-d10	14.611

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	96
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	86
3	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	64
4	Imidazo[1,2-c]pyrimidin-5-ol	135	C6H5N3O	055662-66-3	59
5	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	59





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
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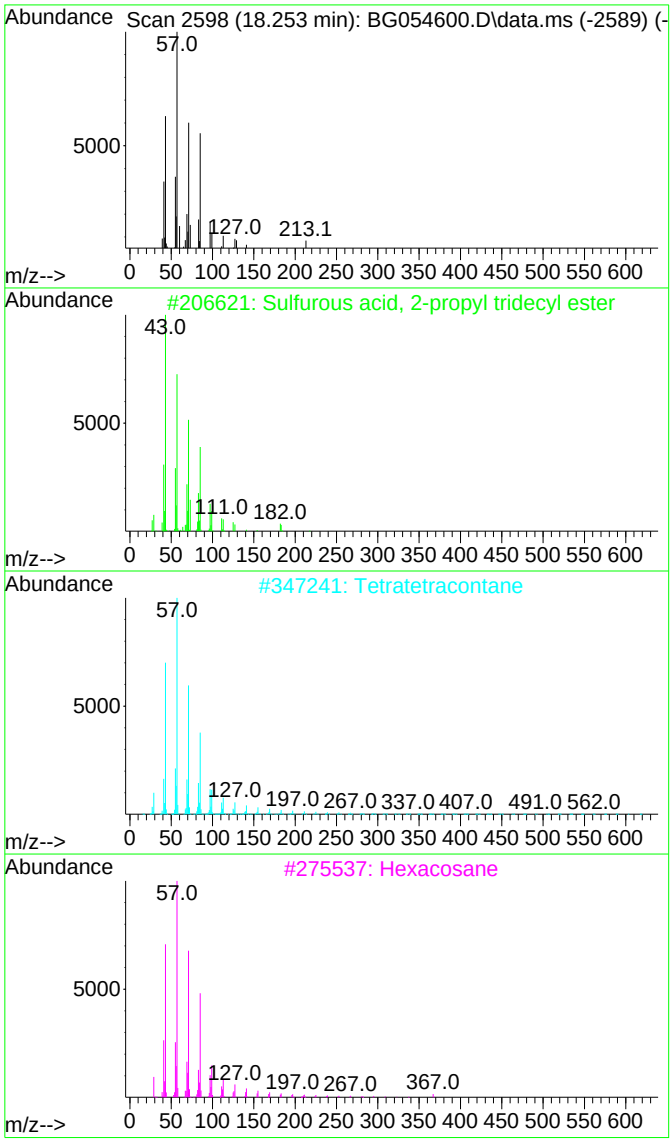
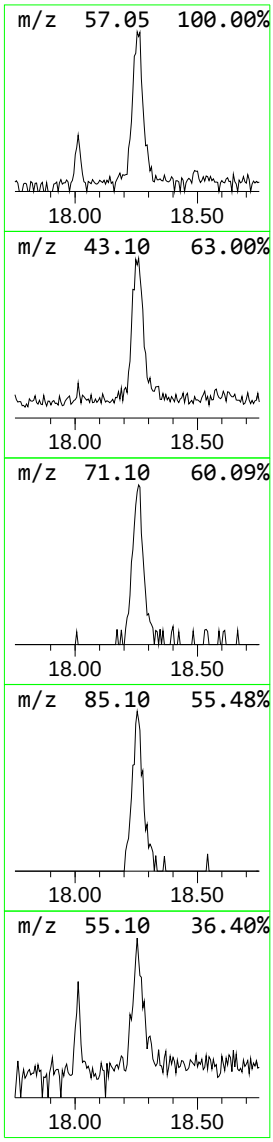
Peak Number 7 Sulfurous acid, 2-propyl tr... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.253	4.28 ng	55200	Phenanthrene-d10	17.360

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	83
2	Tetratetracontane	619	C44H90	007098-22-8	83
3	Hexacosane	366	C26H54	000630-01-3	80
4	Octacosane	394	C28H58	000630-02-4	80
5	Pentacosane	352	C25H52	000629-99-2	72





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TIC Library : C:\Database\NIST20.L
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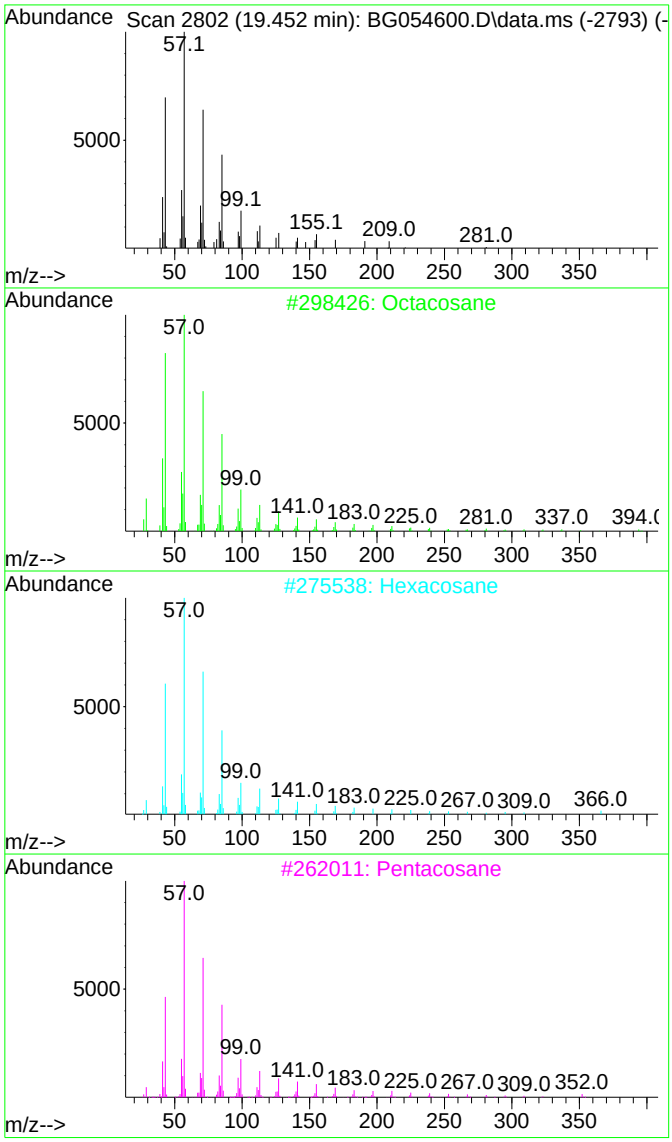
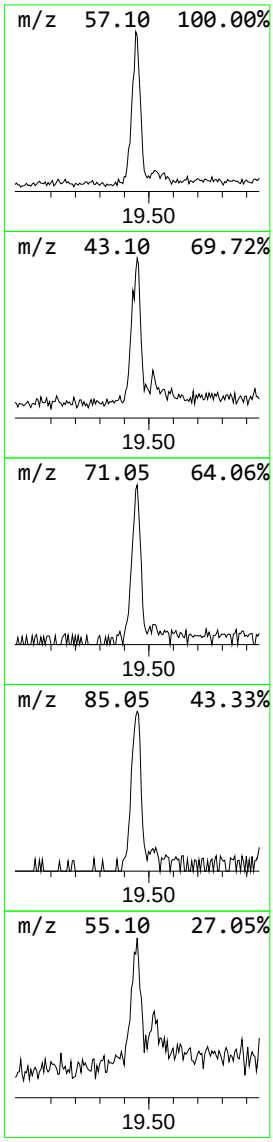
Peak Number 8 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.452	5.23 ng	67516	Phenanthrene-d10	17.360

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	90
2	Hexacosane	366	C26H54	000630-01-3	87
3	Pentacosane	352	C25H52	000629-99-2	87
4	10-Methylnonadecane	282	C20H42	056862-62-5	87
5	Hentriacontane	437	C31H64	000630-04-6	87





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BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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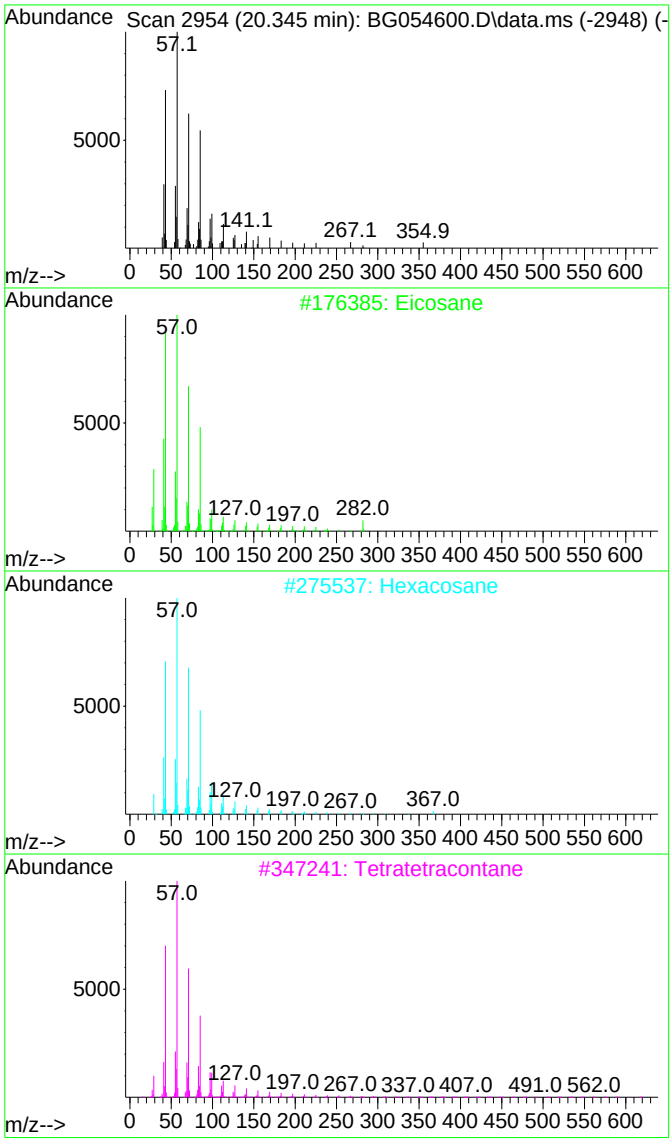
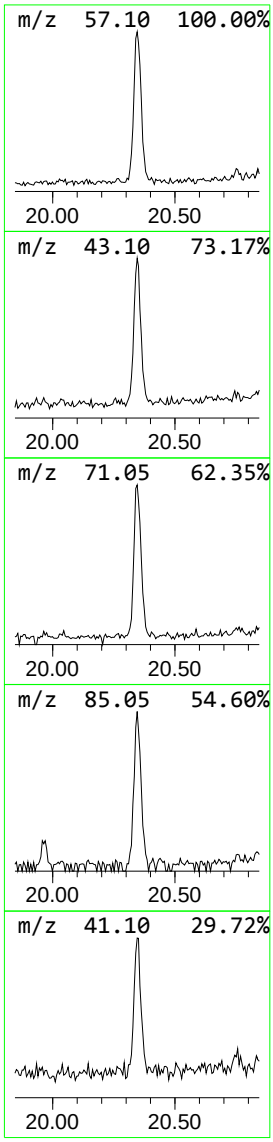
Peak Number 9 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.345	4.44 ng	83998	Chrysene-d12	21.626

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	97
2	Hexacosane	366	C26H54	000630-01-3	91
3	Tetratetracontane	619	C44H90	007098-22-8	91
4	Hentriacontane	437	C31H64	000630-04-6	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





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Acq On : 11 Aug 2022 11:42
Operator : CG/JU
Sample : N3971-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-20R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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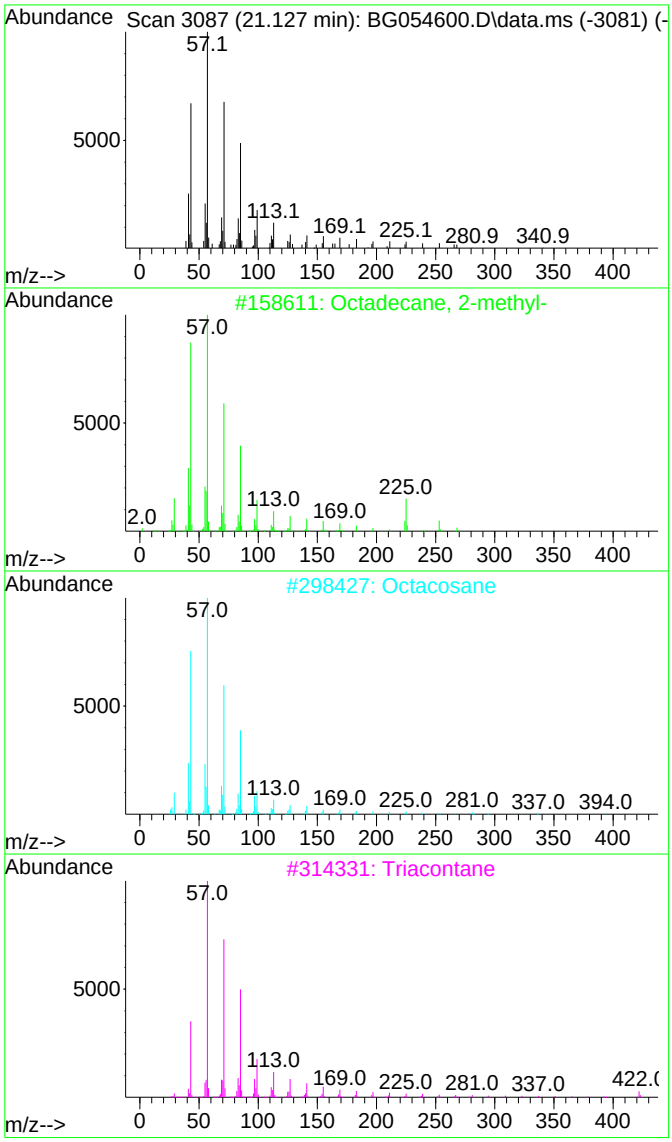
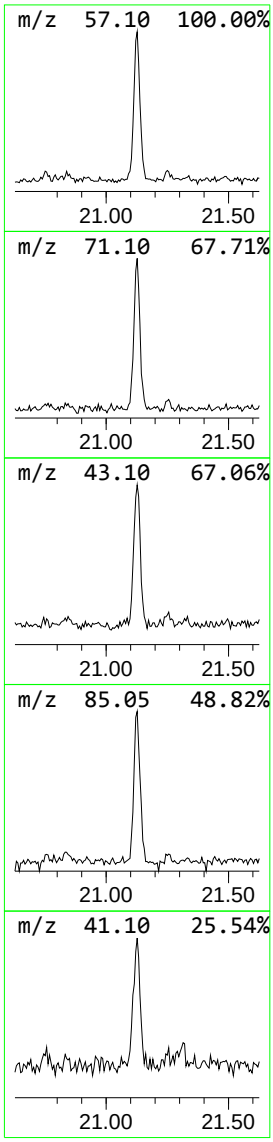
Peak Number 10 Octadecane, 2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.127	4.08 ng	77208	Chrysene-d12	21.626

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 2-methyl-	268	C19H40	001560-88-9	93
2	Octacosane	394	C28H58	000630-02-4	91
3	Triacontane	422	C30H62	000638-68-6	91
4	Docosane	310	C22H46	000629-97-0	91
5	Hentriacontane	437	C31H64	000630-04-6	90





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Acq On : 11 Aug 2022 11:42
Operator : CG/JU
Sample : N3971-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-20R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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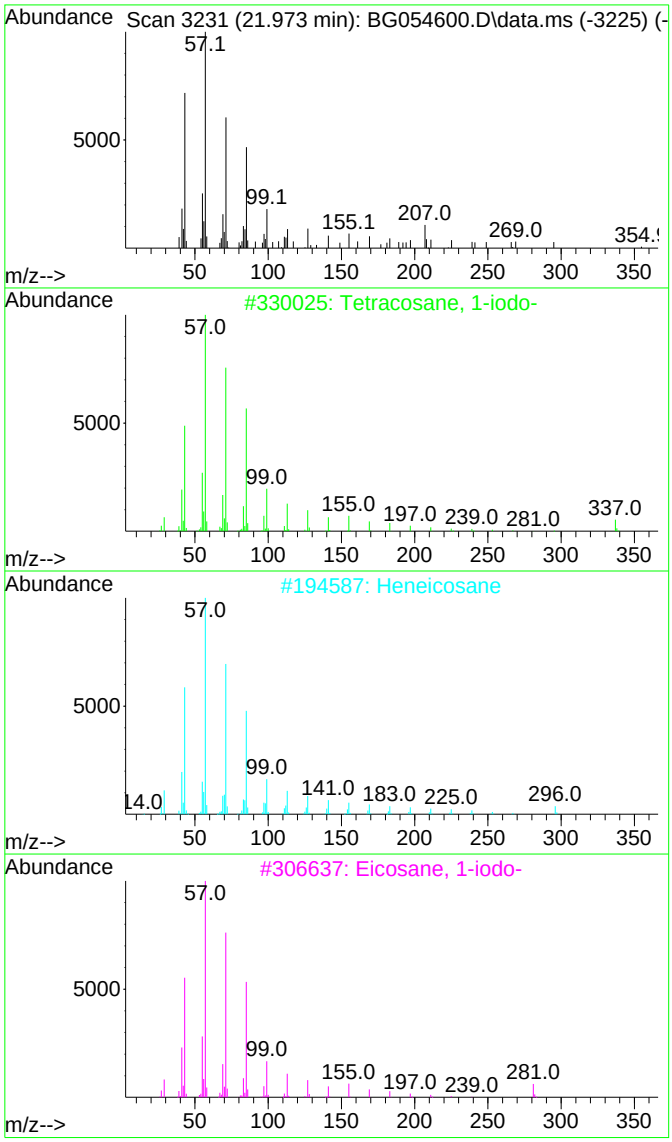
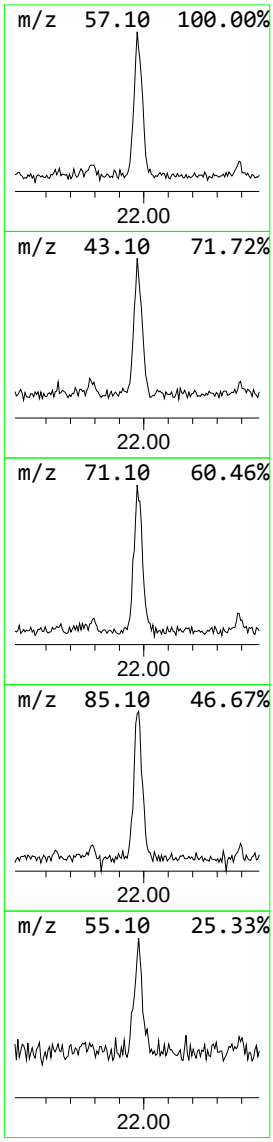
Peak Number 11 Tetracosane, 1-iodo- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.973	4.35 ng	82244	Chrysene-d12	21.626

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	87
2	Heneicosane	296	C21H44	000629-94-7	87
3	Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	83
4	Docosane, 11-butyl-	366	C26H54	013475-76-8	83
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	83





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Data File : BG054600.D
Acq On : 11 Aug 2022 11:42
Operator : CG/JU
Sample : N3971-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-20R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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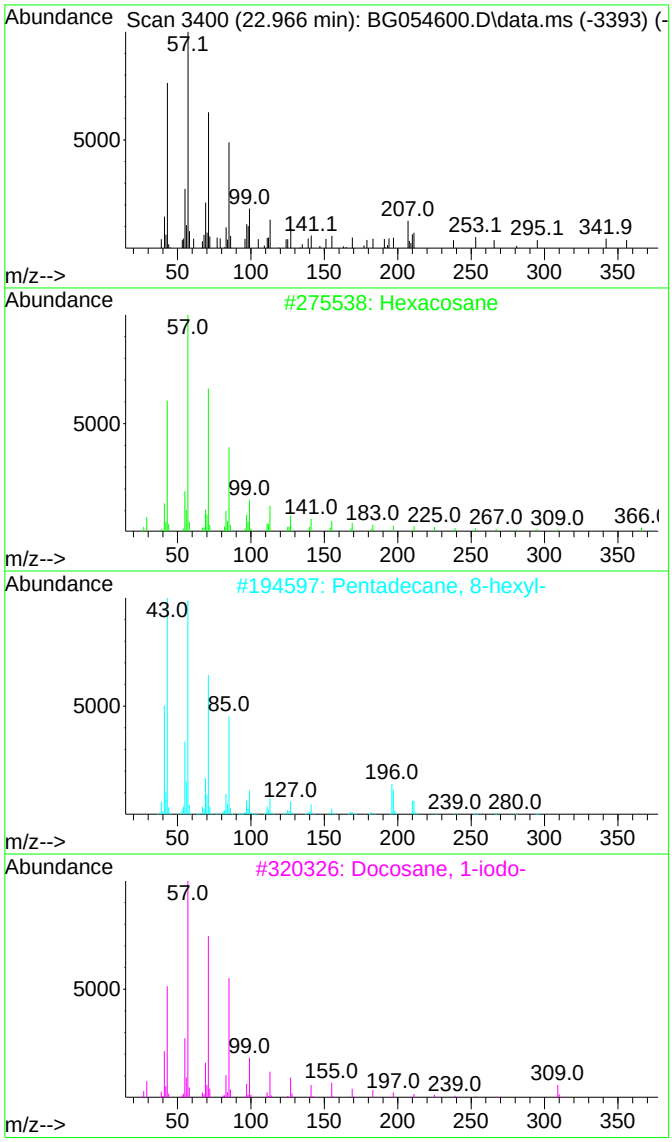
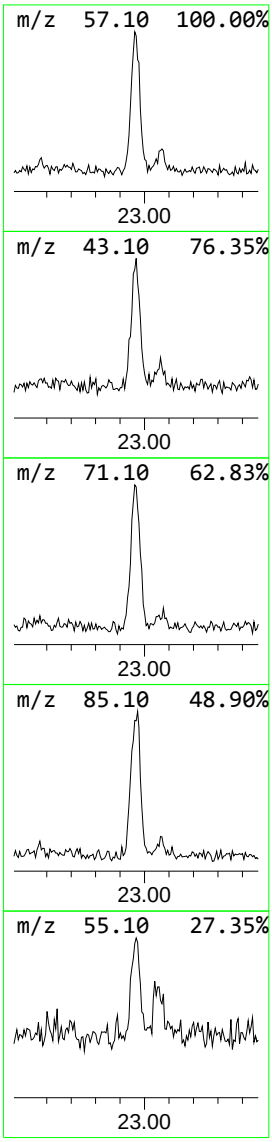
Peak Number 12 Hexacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.965	3.34 ng	63052	Chrysene-d12	21.626

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	58
2	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	58
3	Docosane, 1-iodo-	436	C22H45I	1000406-31-9	53
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	53
5	Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	53





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Data File : BG054600.D
Acq On : 11 Aug 2022 11:42
Operator : CG/JU
Sample : N3971-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-20R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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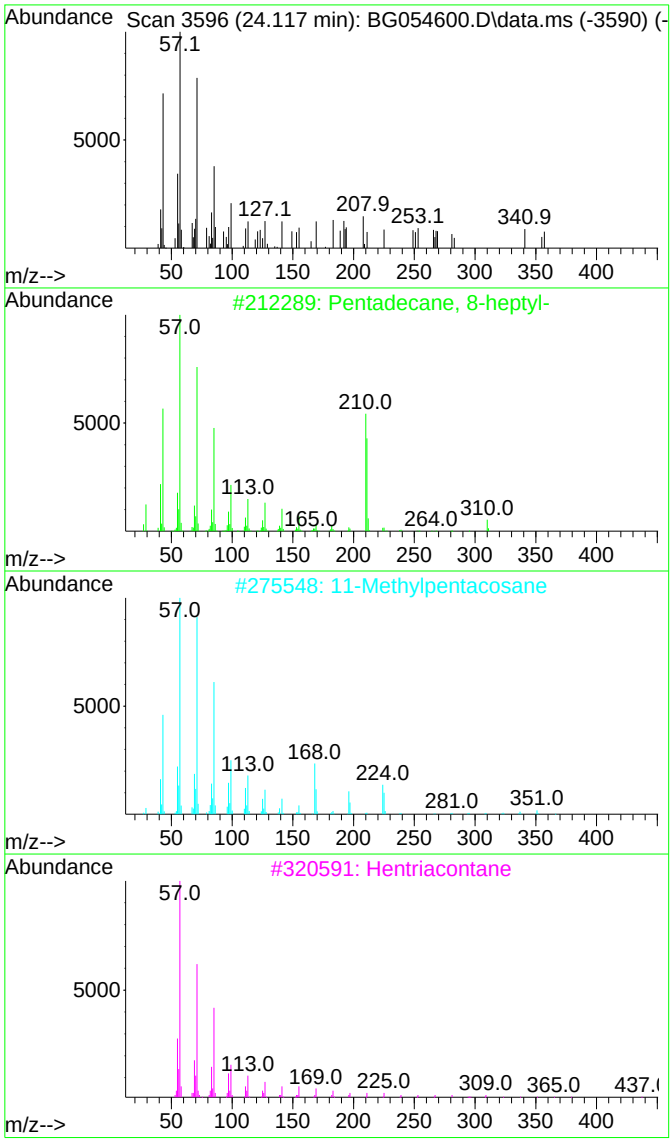
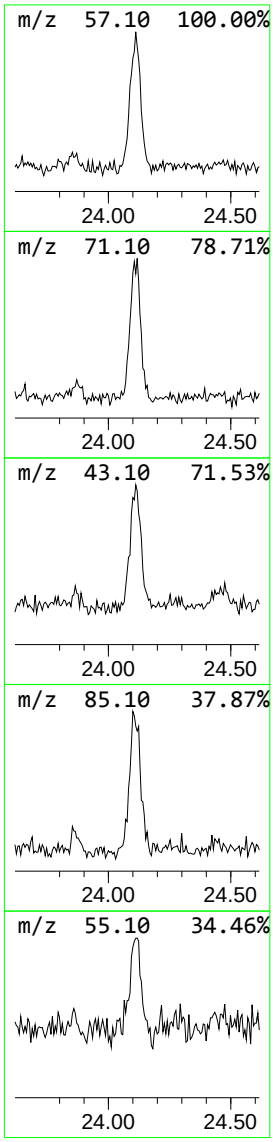
Peak Number 13 Pentadecane, 8-heptyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.117	3.29 ng	64726	Perylene-d12	24.828

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	58
2	11-Methylpentacosane	366	C26H54	015689-71-1	58
3	Hentriacontane	437	C31H64	000630-04-6	58
4	Nonadecane	268	C19H40	000629-92-5	58
5	4-Methylheneicosane	310	C22H46	025117-29-7	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081122\
Data File : BG054600.D
Acq On : 11 Aug 2022 11:42
Operator : CG/JU
Sample : N3971-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-20R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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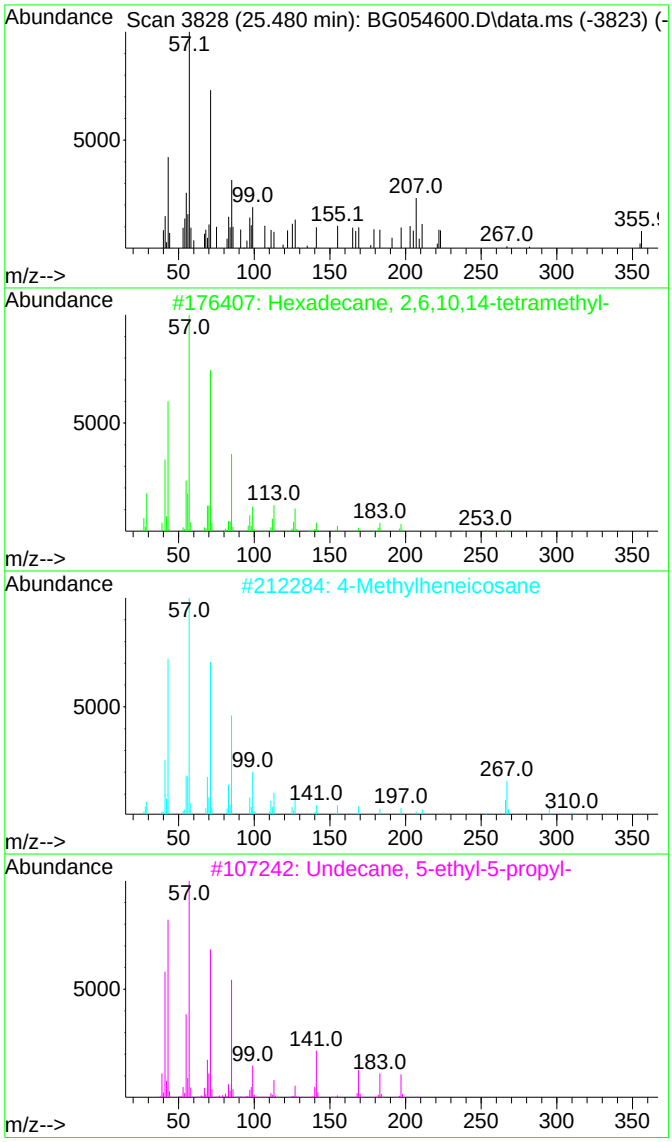
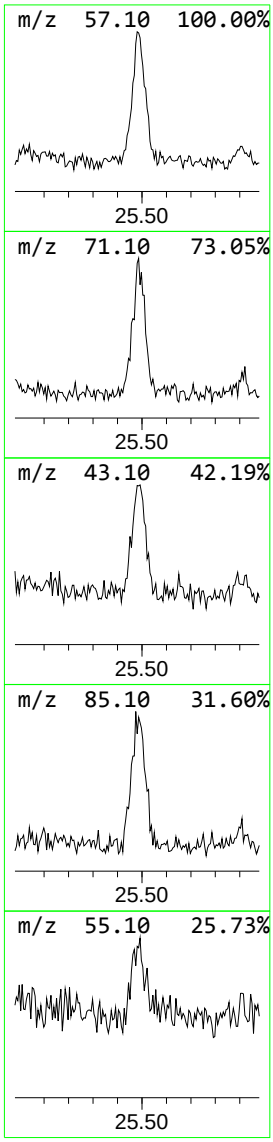
Peak Number 14 unknown25.480 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.480	2.33 ng	45738	Perylene-d12	24.828

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	45
2	4-Methylheneicosane	310	C22H46	025117-29-7	43
3	Undecane, 5-ethyl-5-propyl-	226	C16H34	002755-07-9	43
4	Methoxyacetic acid, 2-tetradecyl...	286	C17H34O3	1000282-04-8	38
5	Undecane, 3,9-dimethyl-	184	C13H28	017301-31-4	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081122\
Data File : BG054600.D
Acq On : 11 Aug 2022 11:42
Operator : CG/JU
Sample : N3971-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-20R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	3.089	97.3	ng	392221	1	7.971	80626	20.0
Cyclopentanone	4.405	22.6	ng	90917	1	7.971	80626	20.0
unknown5.051	5.051	6.6	ng	26501	1	7.971	80626	20.0
2-Propanol, 1-b...	6.602	5.7	ng	22887	1	7.971	80626	20.0
2-Propyl-1-pent...	8.030	6.8	ng	27348	1	7.971	80626	20.0
Phenol, 4-(1,1-...	13.465	25.0	ng	227011	3	14.611	181727	20.0
Sulfurous acid,...	18.253	4.3	ng	55200	4	17.360	257990	20.0
Octacosane	19.452	5.2	ng	67516	4	17.360	257990	20.0
Eicosane	20.345	4.4	ng	83998	5	21.626	378059	20.0
Octadecane, 2-m...	21.127	4.1	ng	77208	5	21.626	378059	20.0
Tetracosane, 1-...	21.973	4.3	ng	82244	5	21.626	378059	20.0
Hexacosane	22.965	3.3	ng	63052	5	21.626	378059	20.0
Pentadecane, 8-...	24.117	3.3	ng	64726	6	24.828	393187	20.0
unknown25.480	25.480	2.3	ng	45738	6	24.828	393187	20.0