LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102221\
Data File : BG050692.D
Acq On : 22 Oct 2021 16:54
Operator : CG/JU
Sample : M4313-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 124027

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-BG100621.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG050692.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.791	385	392	406	rVB	770843	1299120	80.27%	8.188%
2	7.395	656	665	674	rBV	782026	1393452	86.10%	8.782%
3	8.253	804	811	817	rBV	155974	273542	16.90%	1.724%
4	9.422	1001	1010	1021	rBV	466314	862187	53.27%	5.434%
5	10.826	1242	1249	1258	rBV	92801	169407	10.47%	1.068%
6	11.073	1284	1291	1300	rBV	213810	402693	24.88%	2.538%
7	13.494	1696	1703	1710	rVB	740034	1158275	71.57%	7.300%
8	14.869	1931	1937	1943	rVV	312474	503485	31.11%	3.173%
9	14.933	1945	1948	1955	rVB6	10981	19292	1.19%	0.122%
10	16.355	2184	2190	2210	rBV	388376	1019730	63.01%	6.427%
11	17.613	2398	2404	2409	rBV	345254	560317	34.62%	3.531%
12	17.660	2409	2412	2418	rVB	47763	70413	4.35%	0.444%
13	18.465	2545	2549	2559	rVB2	428719	866834	53.56%	5.463%
14	19.722	2759	2763	2781	rVB2	282275	658439	40.68%	4.150%
15	20.204	2839	2845	2850	rVB	959878	1276234	78.86%	8.043%
16	20.697	2923	2929	2939	rVB2	145233	341735	21.12%	2.154%
17	21.473	3055	3061	3066	rBV2	259074	533126	32.94%	3.360%
18	21.543	3068	3073	3078	rVV	394884	710689	43.91%	4.479%
19	21.614	3078	3085	3092	rVB	1036448	1618392	100.00%	10.200%
20	21.720	3094	3103	3117	rVB2	141206	519101	32.08%	3.272%
21	21.913	3130	3136	3142	rVB	323129	557938	34.47%	3.516%
22	22.936	3303	3310	3322	rVB3	137342	421463	26.04%	2.656%
23	25.327	3708	3717	3728	rVB2	208857	631111	39.00%	3.978%

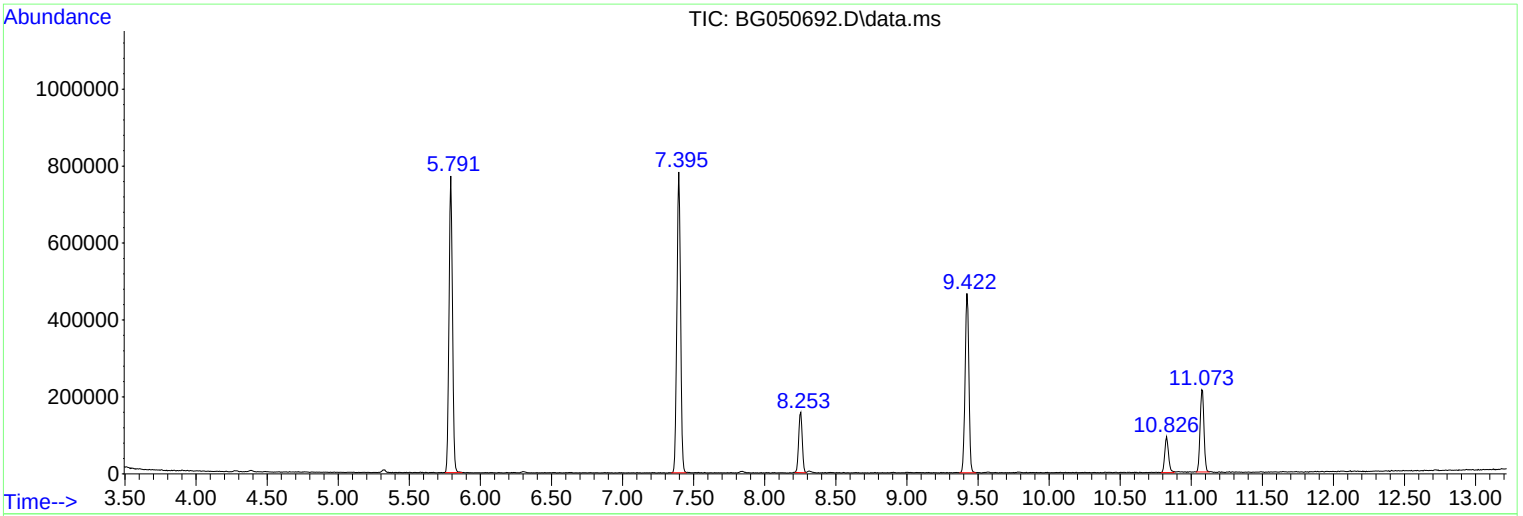
Sum of corrected areas: 15866975

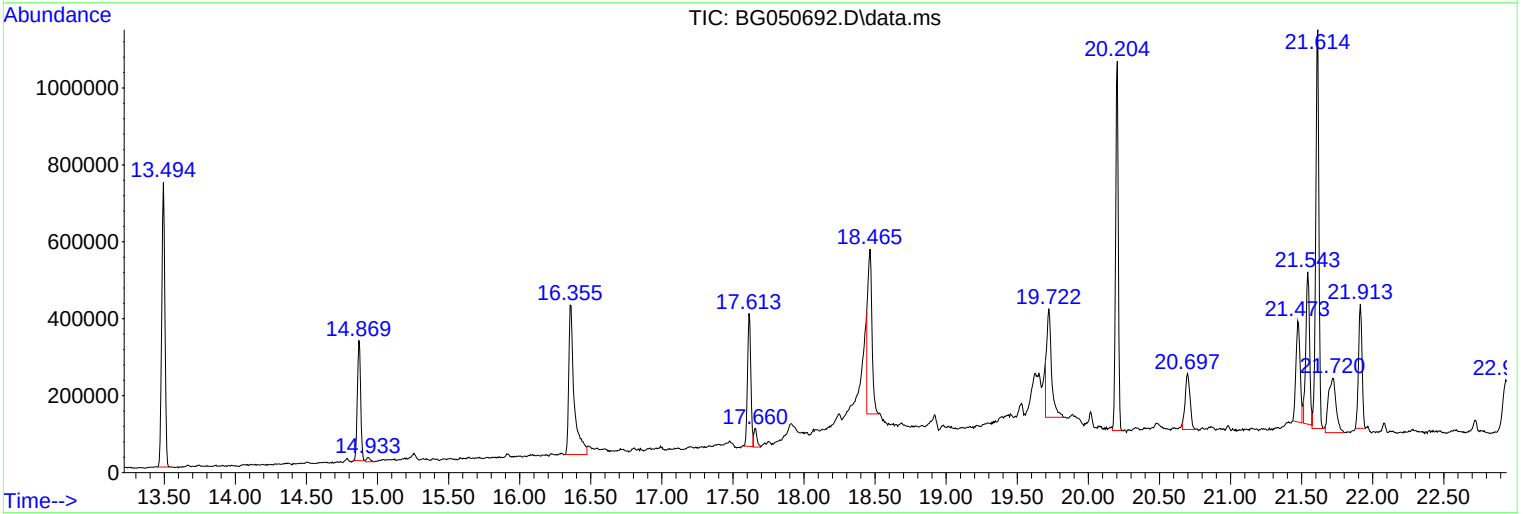
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102221\
Data File : BG050692.D
Acq On : 22 Oct 2021 16:54
Operator : CG/JU
Sample : M4313-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

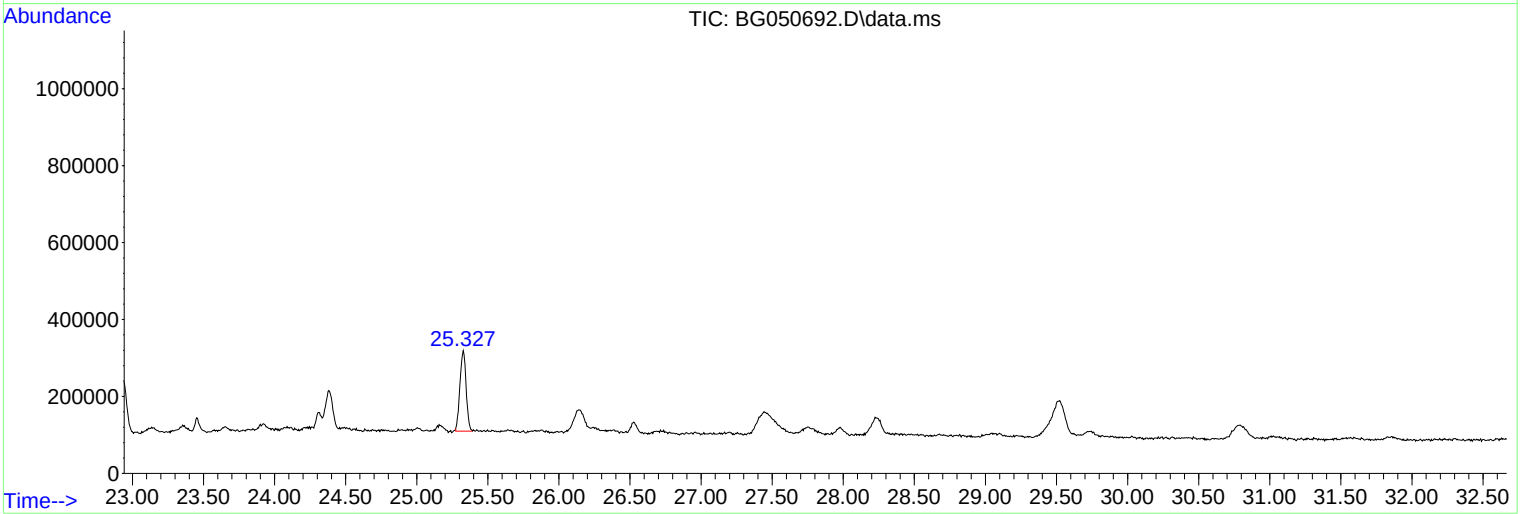
Instrument :
BNA_G
ClientSampleId :
124027

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102221\
Data File : BG050692.D
Acq On : 22 Oct 2021 16:54
Operator : CG/JU
Sample : M4313-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 124027

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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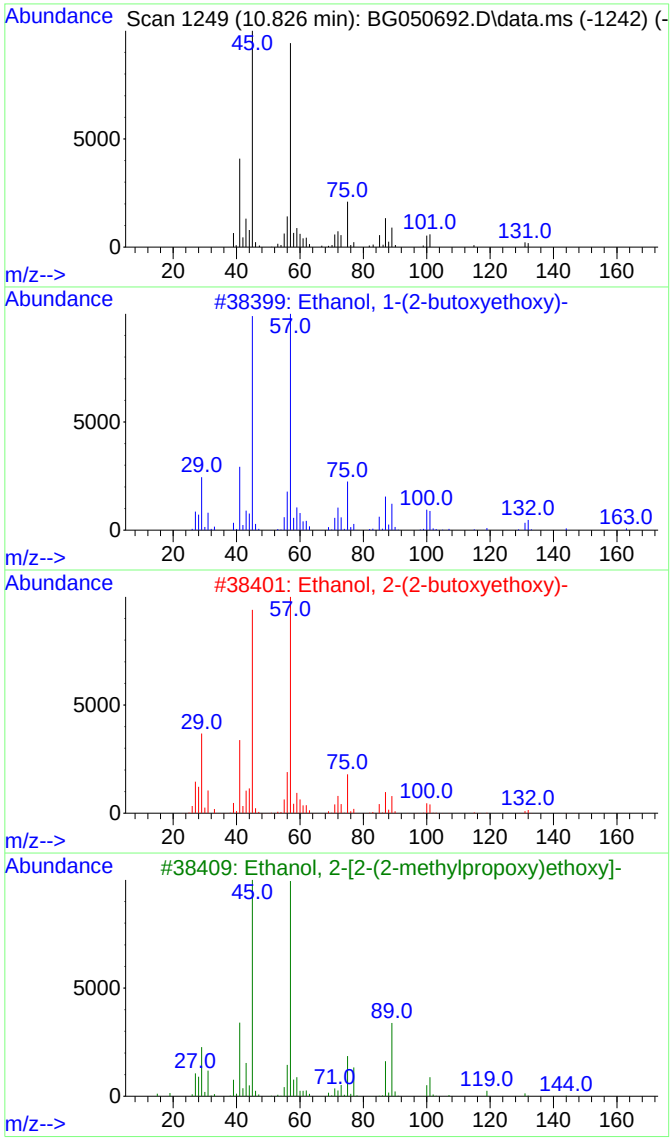
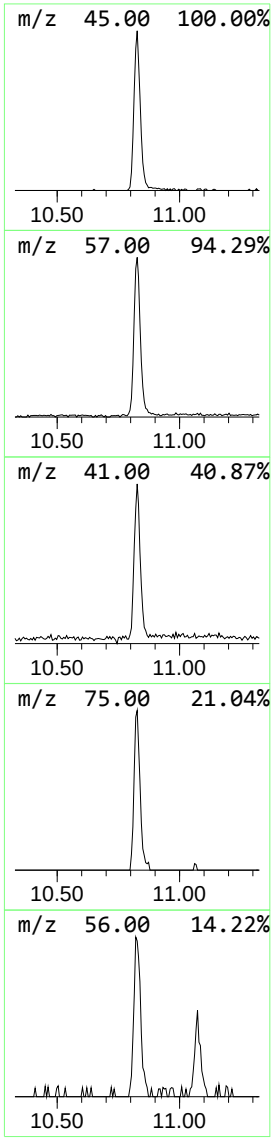
Peak Number 1 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.826	8.41 ng	169407	Naphthalene-d8	11.073

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
2	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	72
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
5	Di-sec-Butyl ether	130	C8H18O	006863-58-7	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102221\
Data File : BG050692.D
Acq On : 22 Oct 2021 16:54
Operator : CG/JU
Sample : M4313-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 124027

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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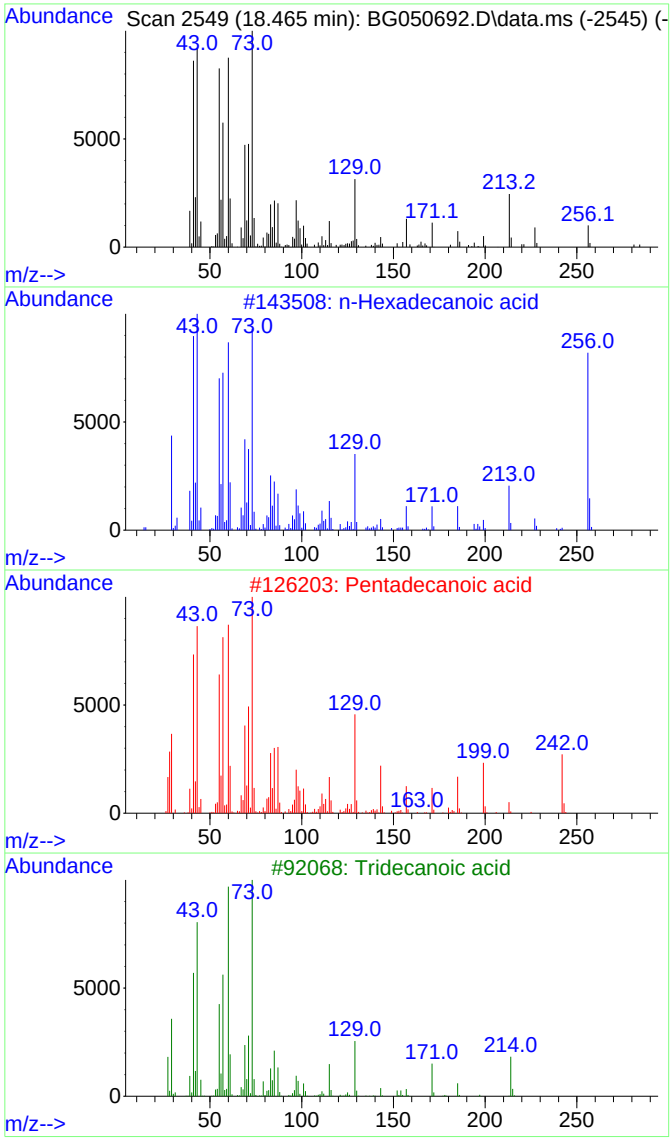
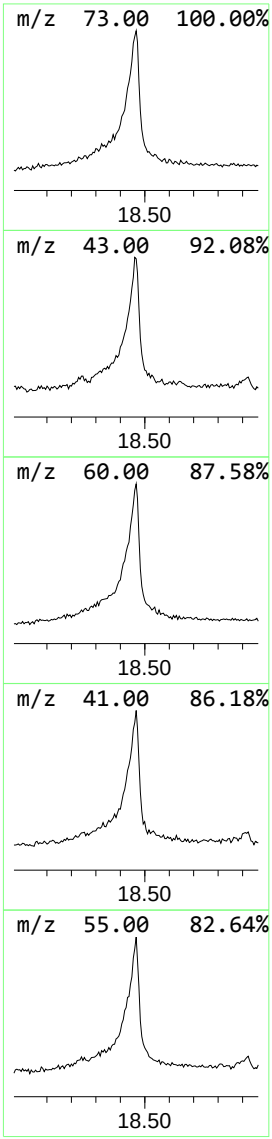
Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.465	30.94 ng	866834	Phenanthrene-d10	17.613

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	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	76
5	Octadecanoic acid	284	C18H36O2	000057-11-4	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102221\
Data File : BG050692.D
Acq On : 22 Oct 2021 16:54
Operator : CG/JU
Sample : M4313-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 124027

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.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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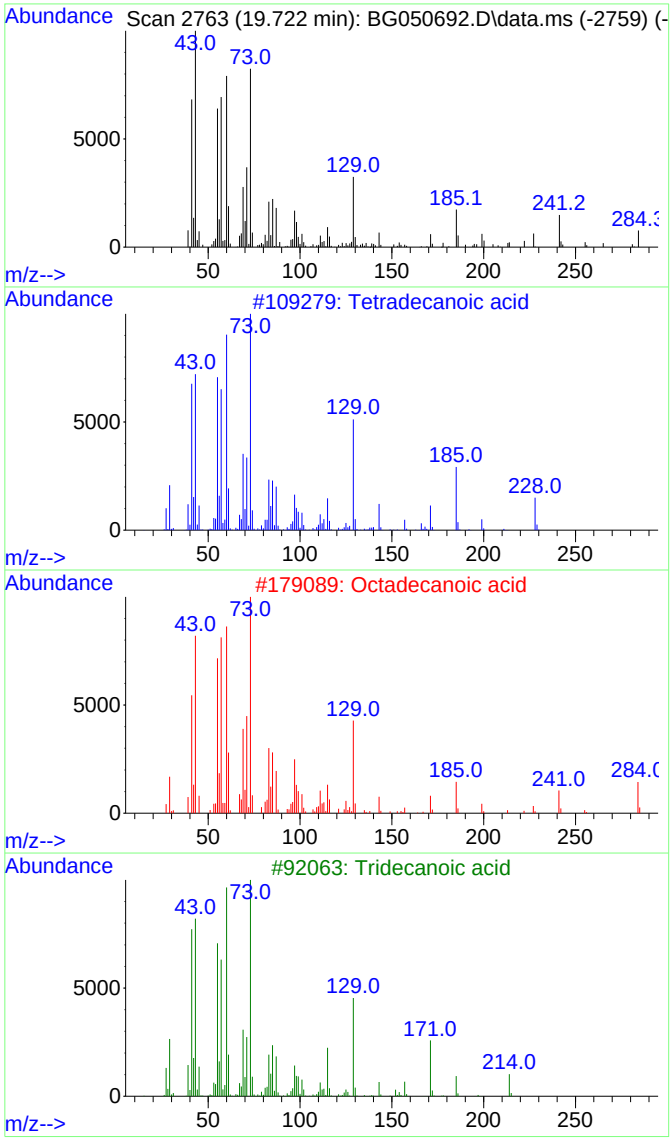
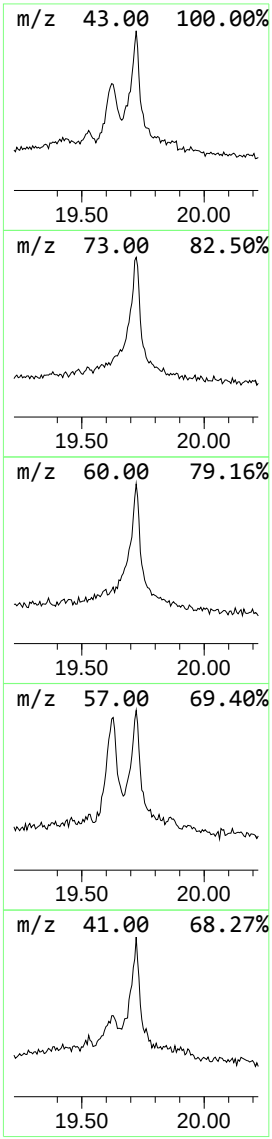
Peak Number 3 Tetradecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.722	23.50 ng	658439	Phenanthrene-d10	17.613

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
2	Octadecanoic acid	284	C18H36O2	000057-11-4	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	80
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	72





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Data File : BG050692.D
Acq On : 22 Oct 2021 16:54
Operator : CG/JU
Sample : M4313-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 124027

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.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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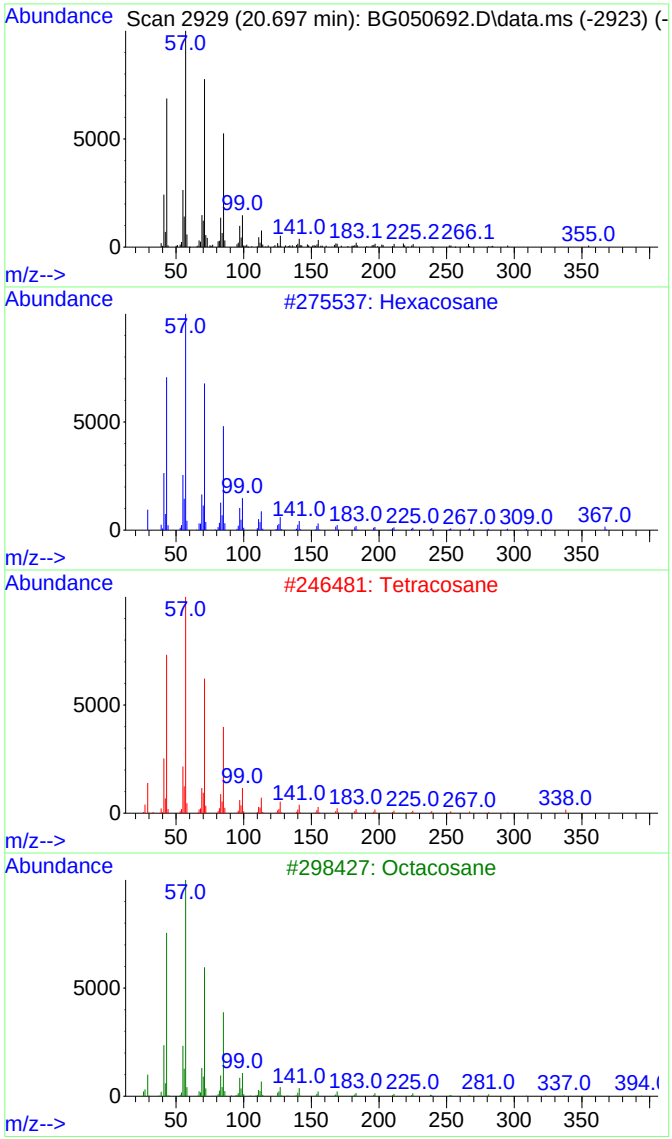
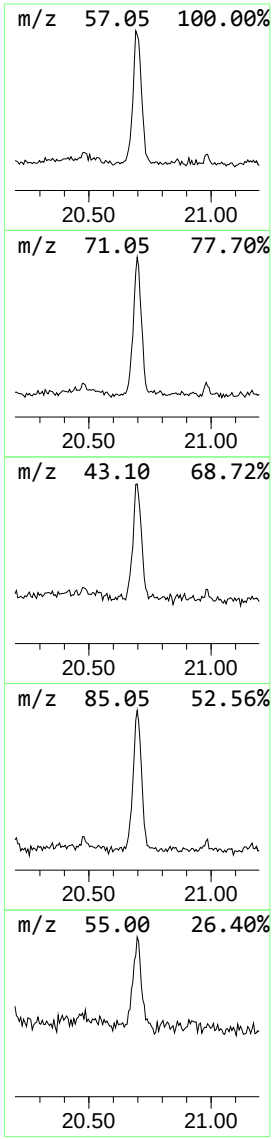
Peak Number 4 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.697	12.25 ng	341735	Chrysene-d12	21.913

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Tetracosane	338	C24H50	000646-31-1	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Eicosane, 9-octyl-	394	C28H58	013475-77-9	91
5	Octadecane	254	C18H38	000593-45-3	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102221\
Data File : BG050692.D
Acq On : 22 Oct 2021 16:54
Operator : CG/JU
Sample : M4313-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 124027

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.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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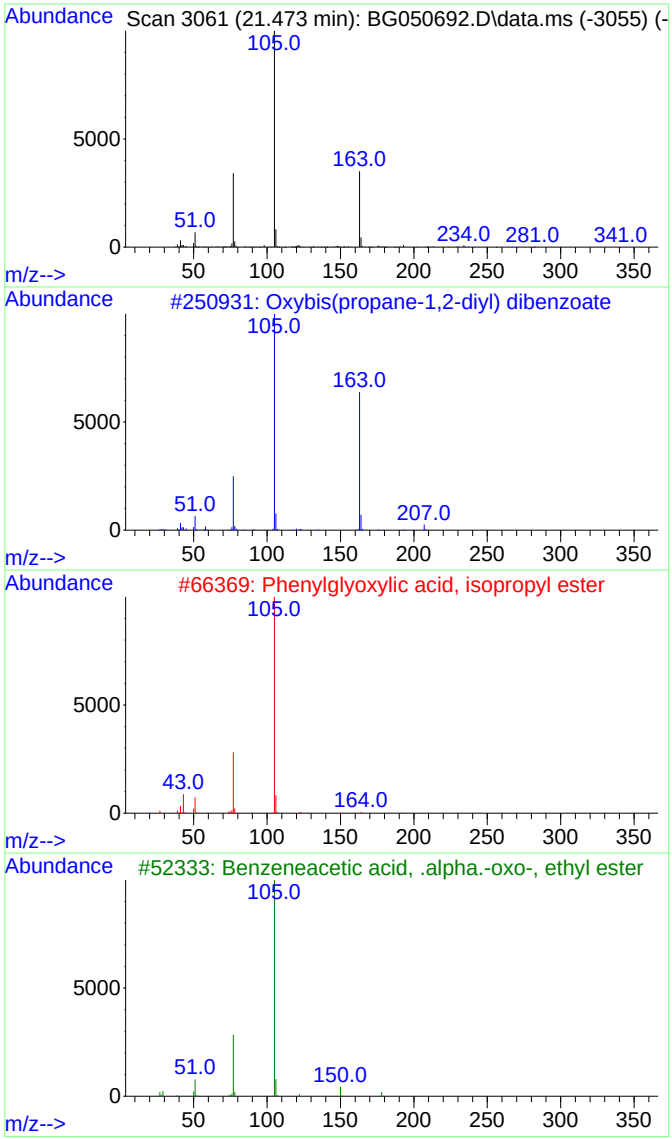
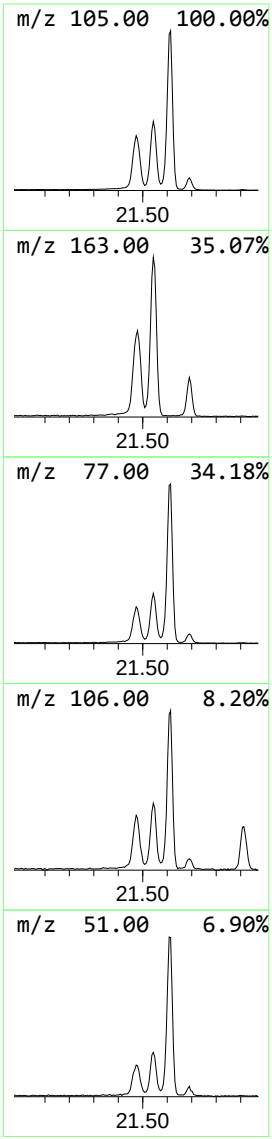
Peak Number 5 unknown21.473 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.473	19.11 ng	533126	Chrysene-d12	21.913

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	50
2	Phenylglyoxylic acid, isopropyl ...	192	C11H12O3	1000453-46-3	47
3	Benzeneacetic acid, .alpha.-oxo-...	178	C10H10O3	001603-79-8	47
4	Benzoic acid, phenyl ester	198	C13H10O2	000093-99-2	47
5	Benzoic acid, 2-propenyl ester	162	C10H10O2	000583-04-0	47





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Operator : CG/JU
Sample : M4313-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 124027

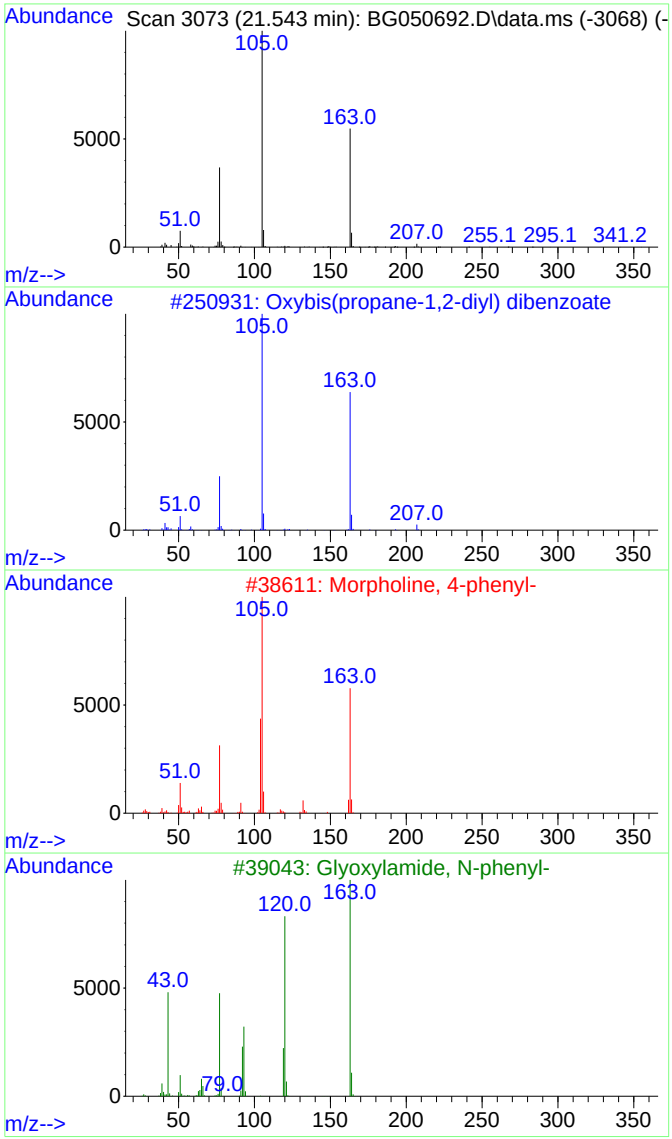
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

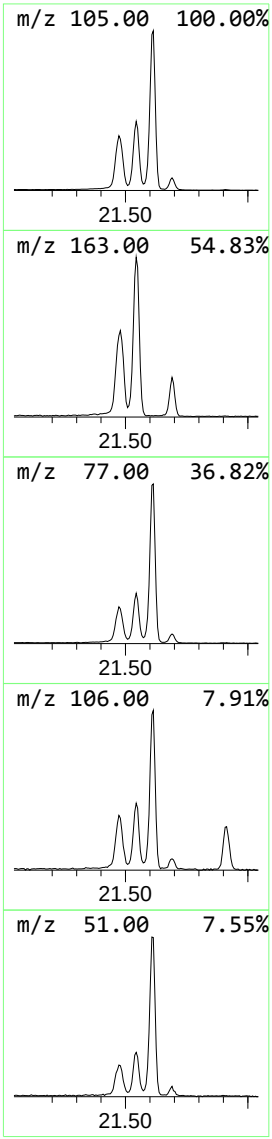
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Oxybis(propane-1,2-diyl) di... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.543	25.48 ng	710689	Chrysene-d12	21.913

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	83
2	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	72
3	Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	50
4	Phenylglyoxylic acid, isopropyl ...	192	C11H12O3	1000453-46-3	38
5	Phenylglyoxylic acid, butyl ester	206	C12H14O3	1000453-46-6	38





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Instrument : BNA_G
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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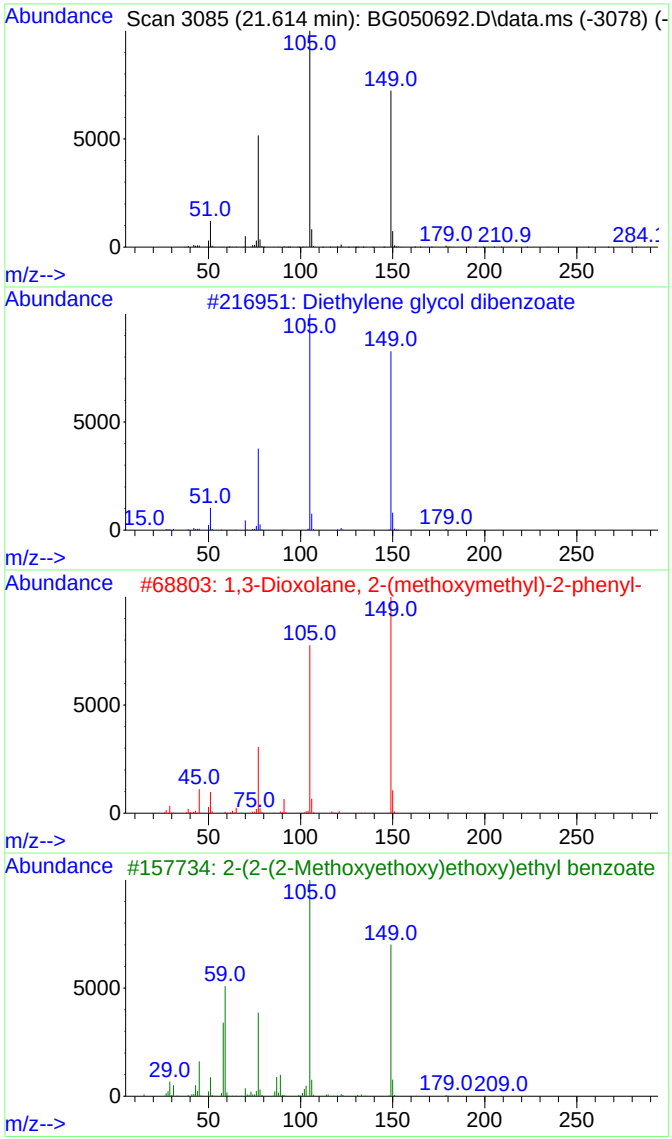
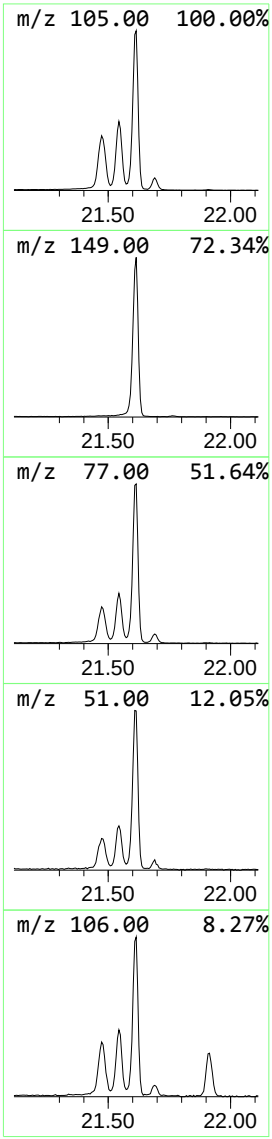
Peak Number 7 Diethylene glycol dibenzoate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.614	58.01 ng	1618390	Chrysene-d12	21.913

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	80
2	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	74
3	2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	74
4	N-[(2-Phenyl-1,3-dioxolan-2-yl)m...	193	C10H11NO3	1000411-48-9	72
5	Phenyl(2-phenyl-1,3-dioxolan-2-y...	298	C18H18O4	006963-16-2	64





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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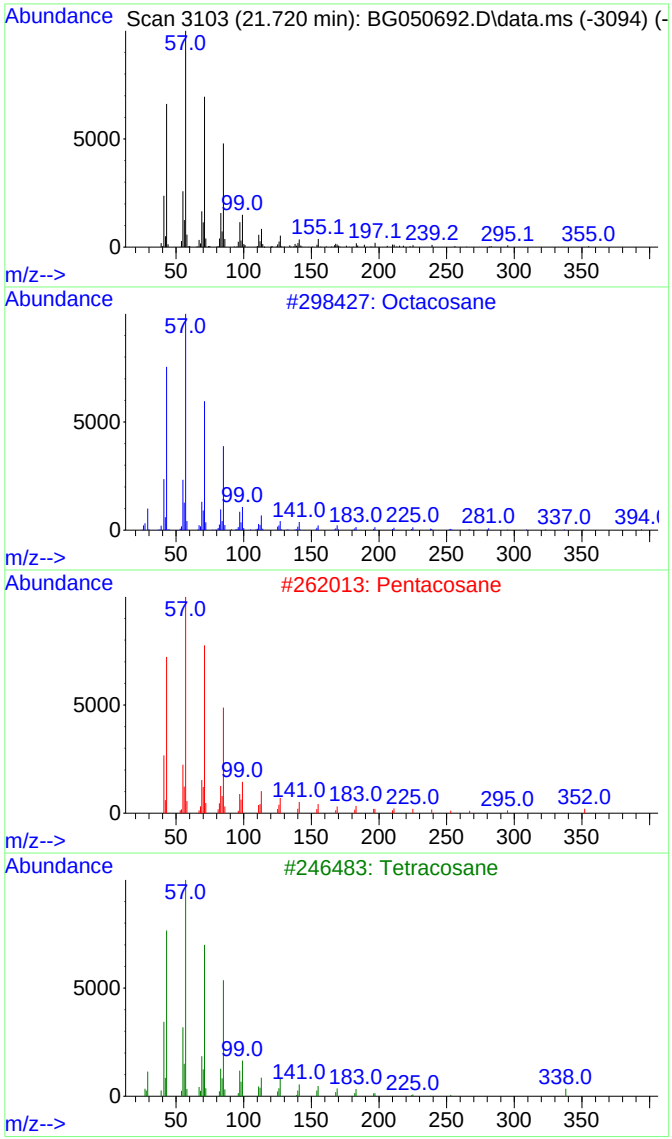
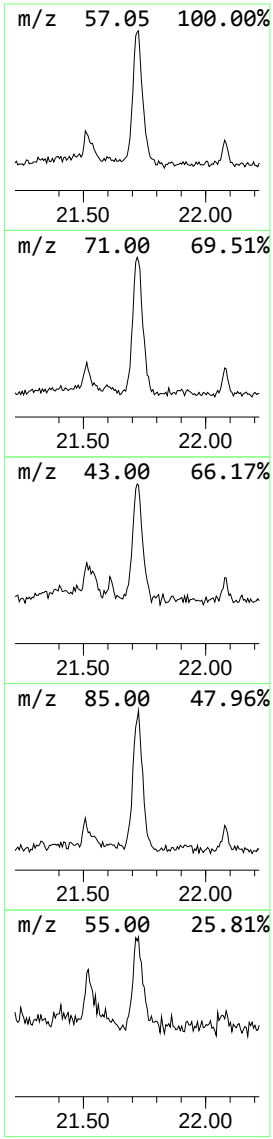
Peak Number 8 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.720	18.61 ng	519101	Chrysene-d12	21.913

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Pentacosane	352	C25H52	000629-99-2	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
5	Heneicosane	296	C21H44	000629-94-7	90





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Operator : CG/JU
Sample : M4313-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 124027

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.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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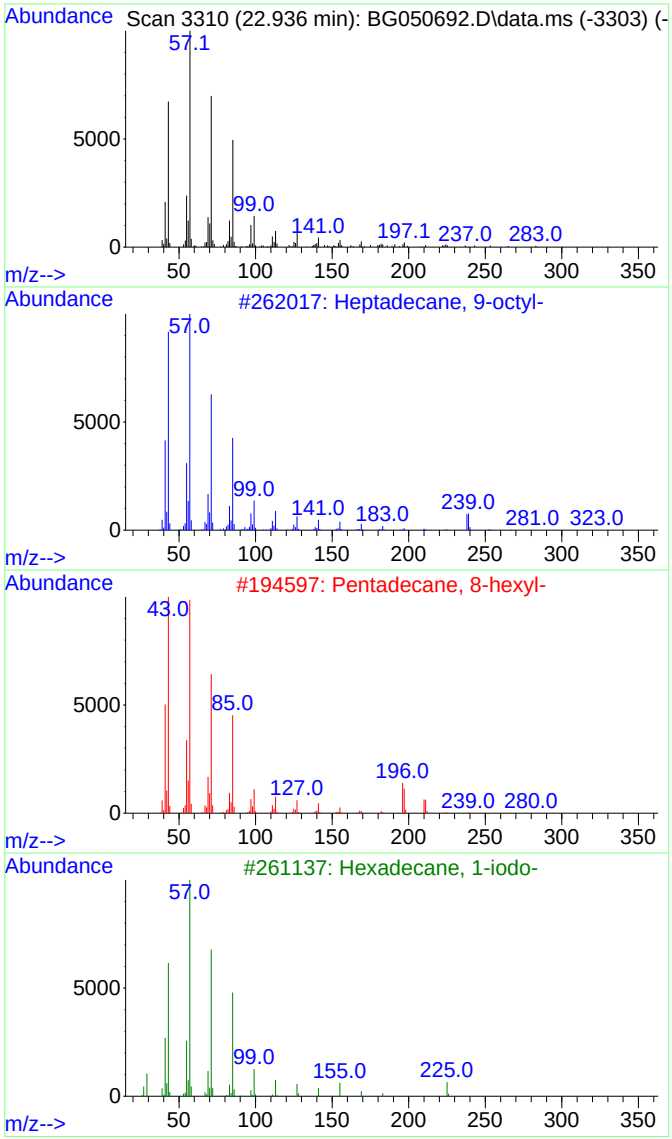
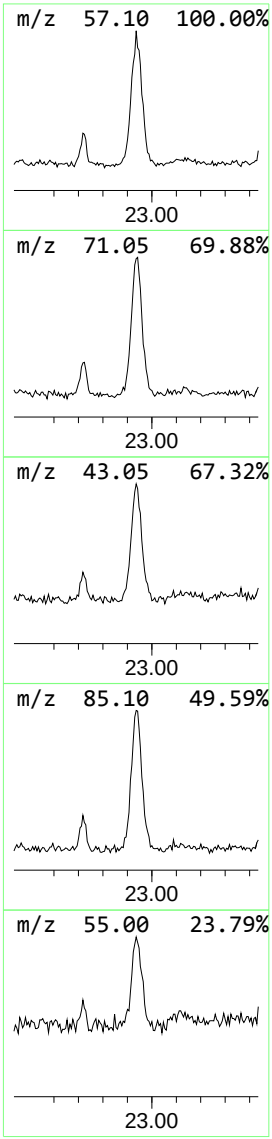
Peak Number 9 Heptadecane, 9-octyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.936	15.11 ng	421463	Chrysene-d12	21.913

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	90
3	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	86
4	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86
5	Heneicosane	296	C21H44	000629-94-7	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102221\
Data File : BG050692.D
Acq On : 22 Oct 2021 16:54
Operator : CG/JU
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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Ethanol, 1-(2-b...	10.826	8.4	ng	169407	2	11.073	402693	20.0
n-Hexadecanoic ...	18.465	30.9	ng	866834	4	17.613	560317	20.0
Tetradecanoic acid	19.722	23.5	ng	658439	4	17.613	560317	20.0
Hexacosane	20.697	12.3	ng	341735	5	21.913	557938	20.0
unknown21.473	21.473	19.1	ng	533126	5	21.913	557938	20.0
Oxybis(propane-...	21.543	25.5	ng	710689	5	21.913	557938	20.0
Diethylene glyc...	21.614	58.0	ng	1618390	5	21.913	557938	20.0
Octacosane	21.720	18.6	ng	519101	5	21.913	557938	20.0
Heptadecane, 9-...	22.936	15.1	ng	421463	5	21.913	557938	20.0