LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG011918\
Data File : BG032163.D
Acq On : 19 Jan 2018 22:14
Operator : SJ/JU
Sample : J1205-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-3

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:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	6.166	484	490	504	rVB	161981	284693	11.18%	2.451%
2	7.847	768	776	787	rBV2	102886	220418	8.66%	1.897%
3	8.252	837	845	857	rBV	302329	568802	22.35%	4.896%
4	8.740	921	928	939	rVB	115229	214194	8.42%	1.844%
5	9.075	978	985	998	rBB	311293	586140	23.03%	5.045%
6	9.938	1122	1132	1146	rBB	219699	404908	15.91%	3.485%
7	11.624	1412	1419	1428	rVB	151487	291612	11.46%	2.510%
8	14.004	1817	1824	1835	rVB	785218	1261367	49.56%	10.857%
9	14.803	1952	1960	1966	rBV	84412	140040	5.50%	1.205%
10	15.220	2025	2031	2035	rBV	31233	46028	1.81%	0.396%
11	15.379	2048	2058	2065	rBV2	255159	448487	17.62%	3.860%
12	16.160	2178	2191	2196	rBV3	42435	70691	2.78%	0.608%
13	16.560	2251	2259	2264	rBV6	21761	51596	2.03%	0.444%
14	16.848	2302	2308	2324	rVB	681808	1093812	42.97%	9.415%
15	17.018	2332	2337	2347	rBV5	34540	87609	3.44%	0.754%
16	17.471	2407	2414	2420	rBV3	21091	36576	1.44%	0.315%
17	18.111	2516	2523	2531	rBV	429143	680299	26.73%	5.856%
18	18.928	2657	2662	2669	rBV	144916	224018	8.80%	1.928%
19	20.167	2868	2873	2880	rBV2	84482	126554	4.97%	1.089%
20	20.643	2948	2954	2961	rBV	1846935	2545367	100.00%	21.909%
21	21.983	3177	3182	3192	rBV2	96871	168722	6.63%	1.452%
22	22.447	3251	3261	3272	rBV	541725	1019050	40.04%	8.771%
23	24.321	3573	3580	3587	rVB6	11339	27918	1.10%	0.240%
24	26.143	3877	3890	3908	rVB	314366	1018848	40.03%	8.770%

Sum of corrected areas: 11617749

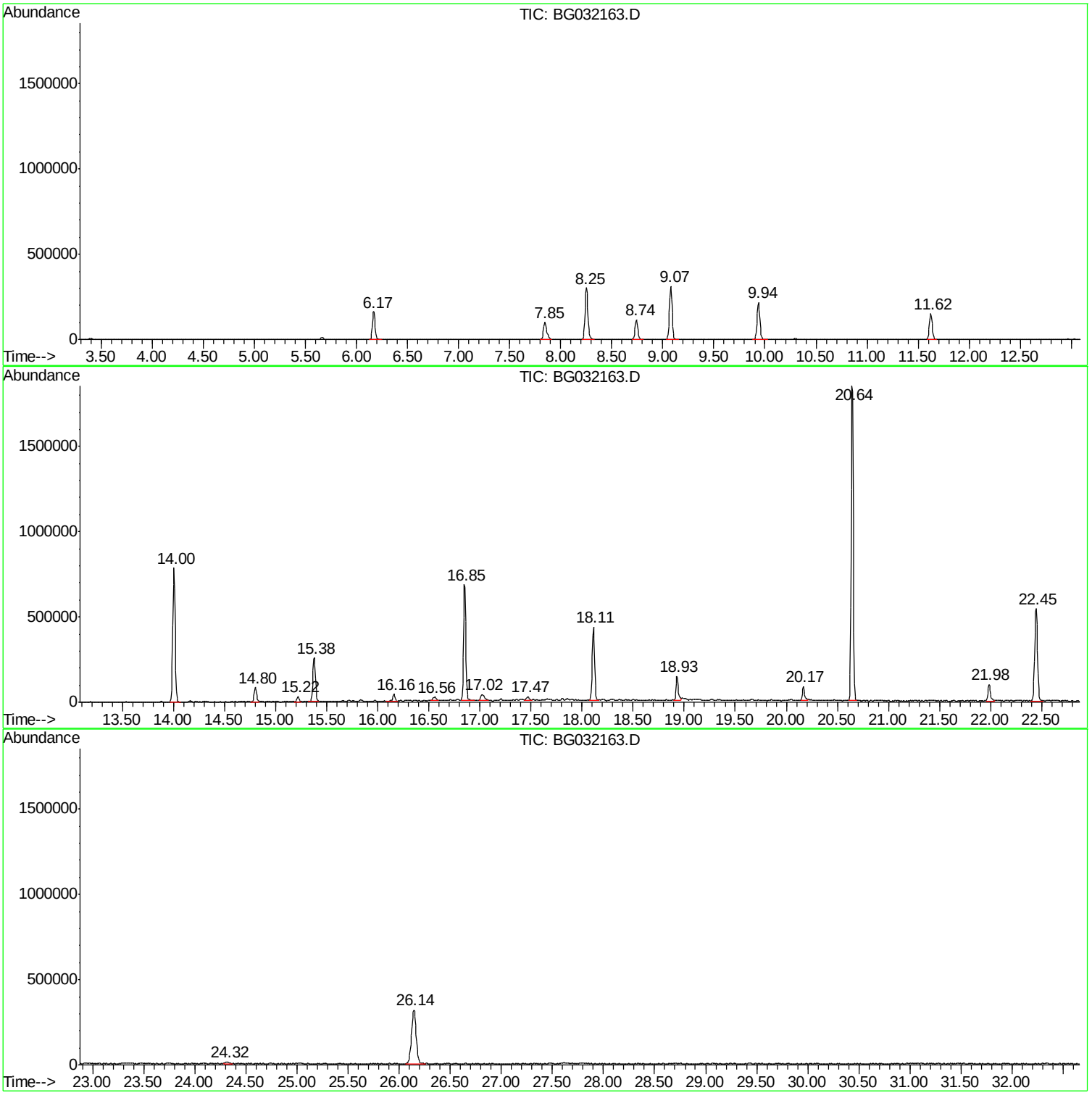
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA G\DATA\BG011918\
Data File : BG032163.D
Acq On : 19 Jan 2018 22:14
Operator : SJ/JU
Sample : J1205-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-3

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA G\DATA\BG011918\
Data File : BG032163.D
Acq On : 19 Jan 2018 22:14
Operator : SJ/JU
Sample : J1205-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

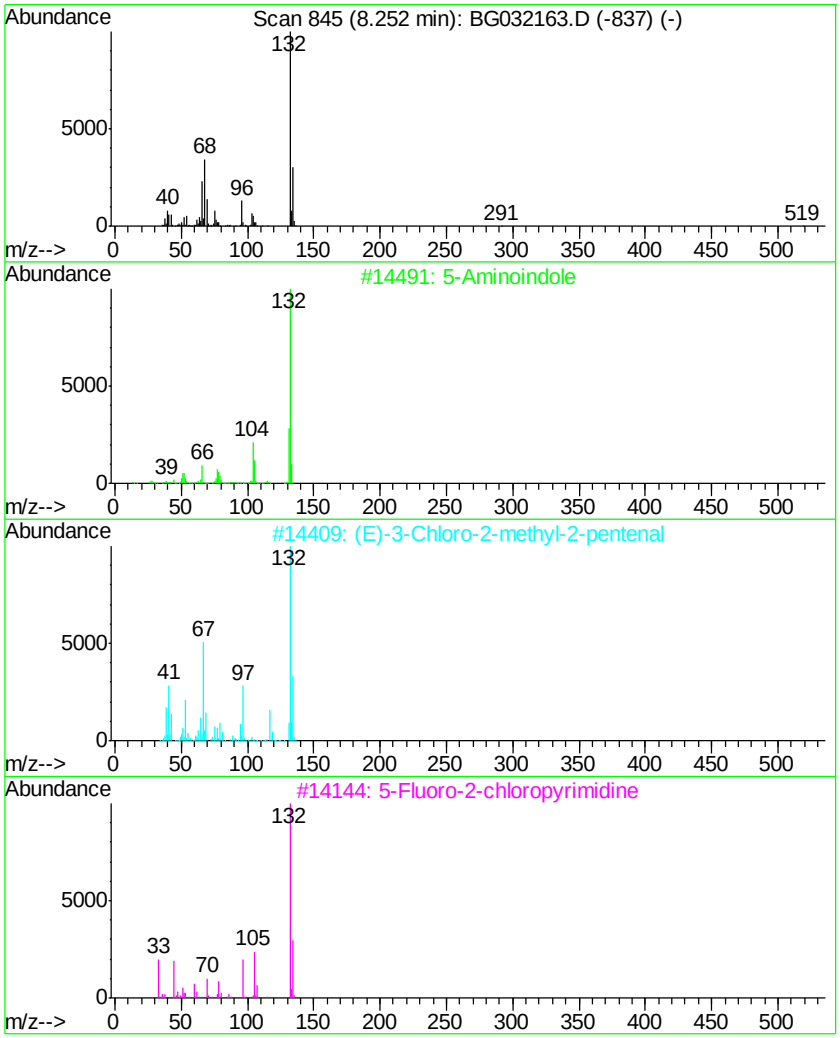
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

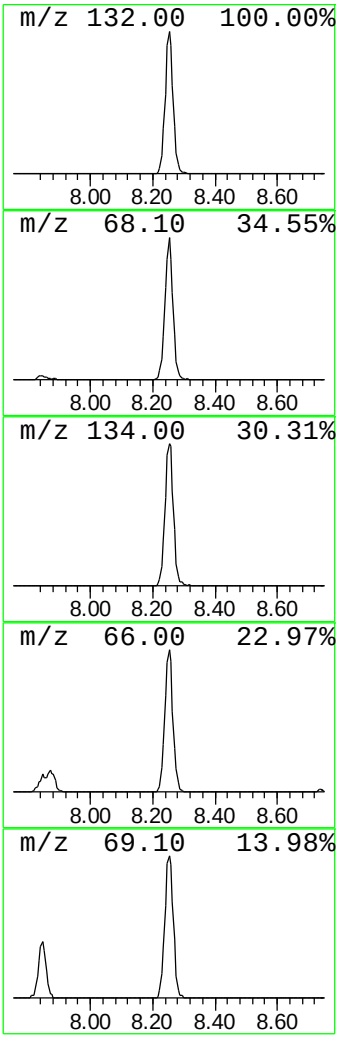
****

Peak Number 1 5-Aminoindole Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.25	53.11 ng	568802	1,4-Dichlorobenzene-d4	8.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminoindole	132	C8H8N2	005192-03-0	22
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	17
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	12
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG011918\
Data File : BG032163.D
Acq On : 19 Jan 2018 22:14
Operator : SJ/JU
Sample : J1205-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.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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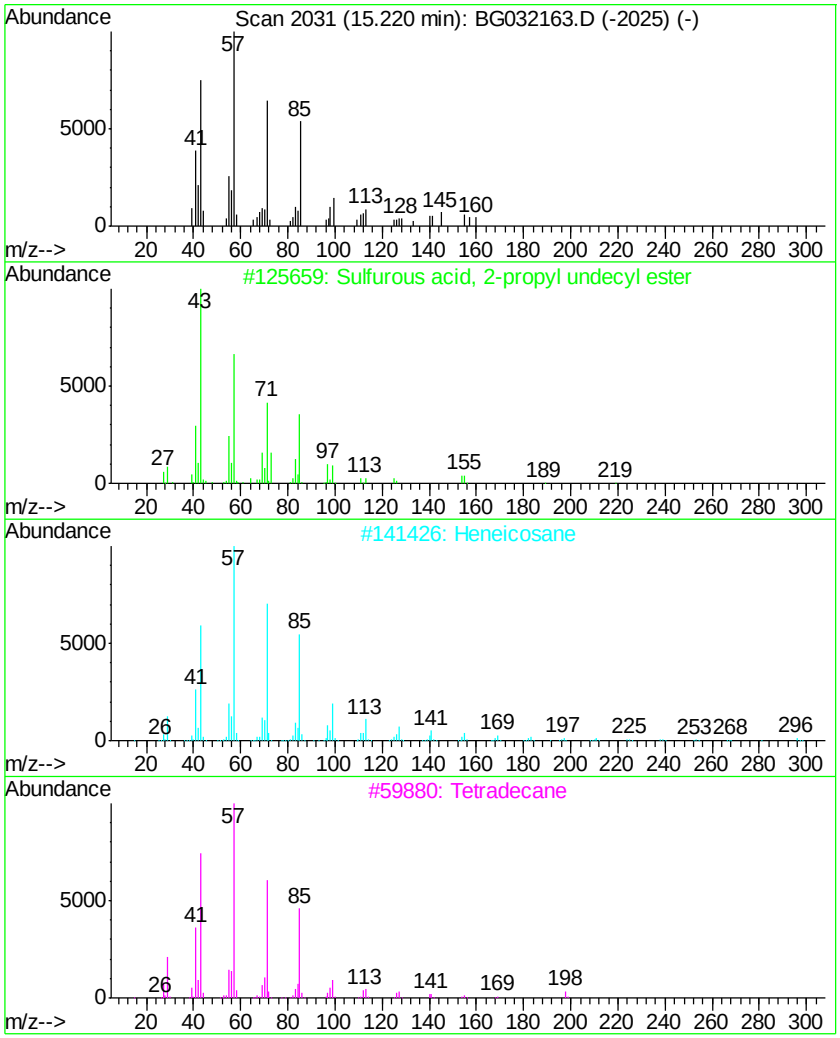
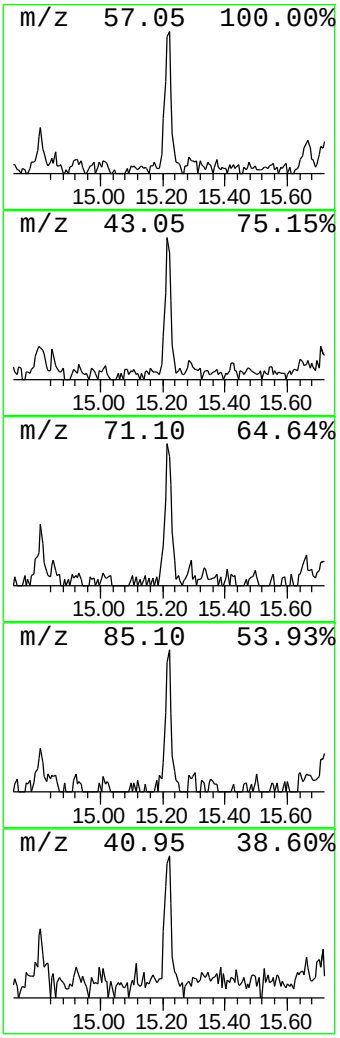
Peak Number 3 Sulfurous acid, 2-propyl un... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.22	2.05 ng	46028	Acenaphthene-d10	15.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, 2-propyl undecyl...	278	C14H30O3S	1000309-12-2	72
2	Heneicosane	296	C21H44	000629-94-7	64
3	Tetradecane	198	C14H30	000629-59-4	59
4	2-methyloctacosane	408	C29H60	1000376-72-8	53
5	Tridecane, 4-methyl-	198	C14H30	026730-12-1	53





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Data File : BG032163.D
Acq On : 19 Jan 2018 22:14
Operator : SJ/JU
Sample : J1205-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.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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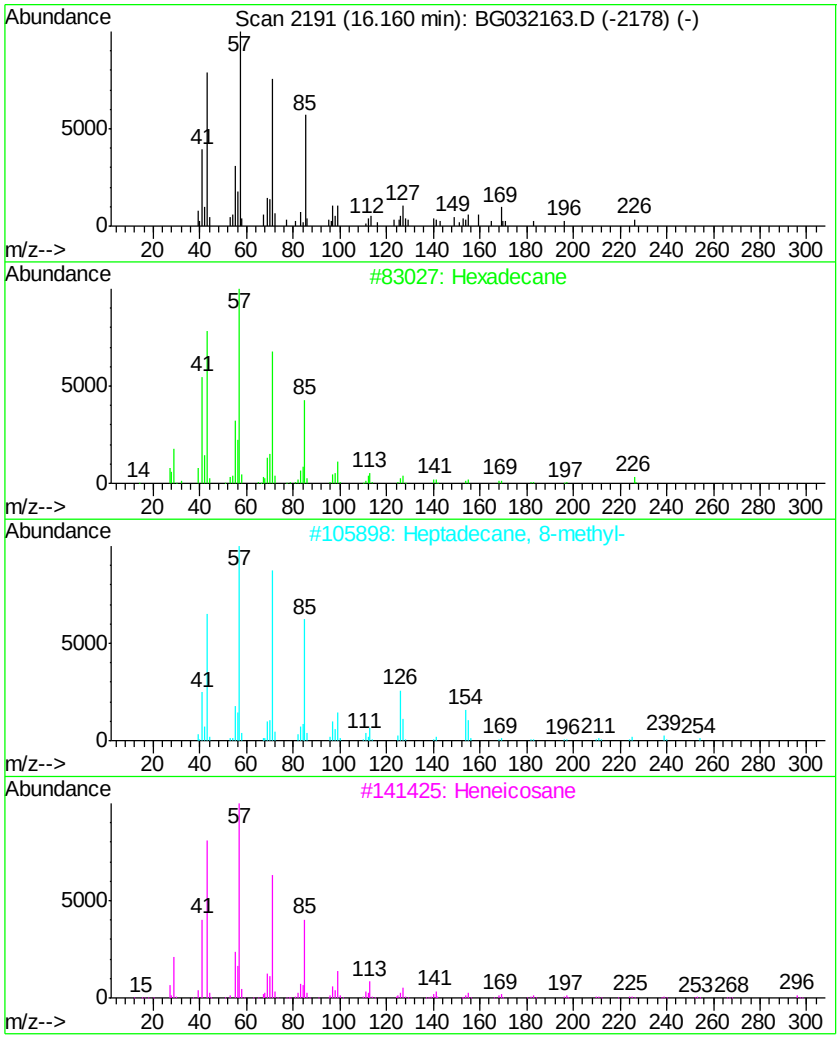
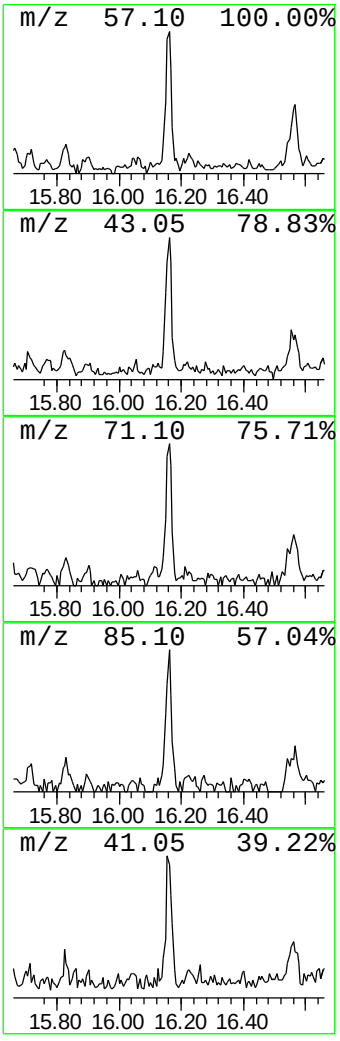
Peak Number 4 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.16	3.15 ng	70691	Acenaphthene-d10	15.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Heptadecane, 8-methyl-	254	C18H38	013287-23-5	86
3	Heneicosane	296	C21H44	000629-94-7	80
4	Heptadecane	240	C17H36	000629-78-7	80
5	Dodecane	170	C12H26	000112-40-3	72





Data Path : Z:\HPCHEM1\BNA G\DATA\BG011918\
Data File : BG032163.D
Acq On : 19 Jan 2018 22:14
Operator : SJ/JU
Sample : J1205-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.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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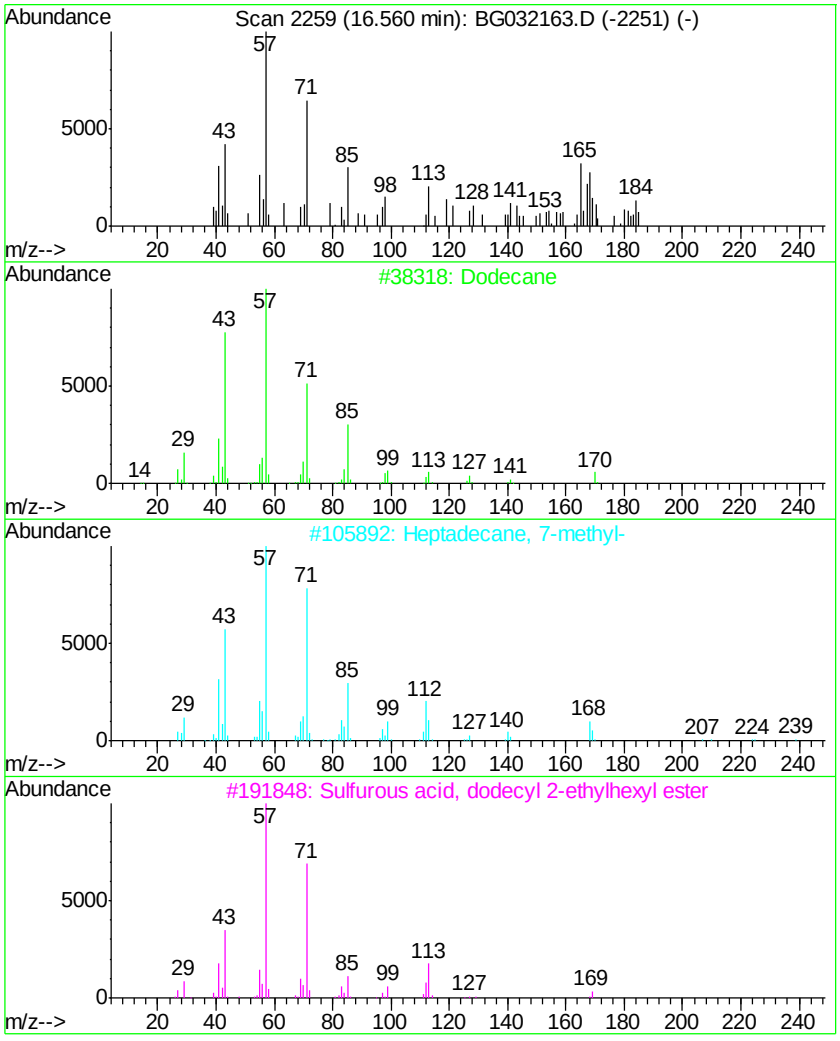
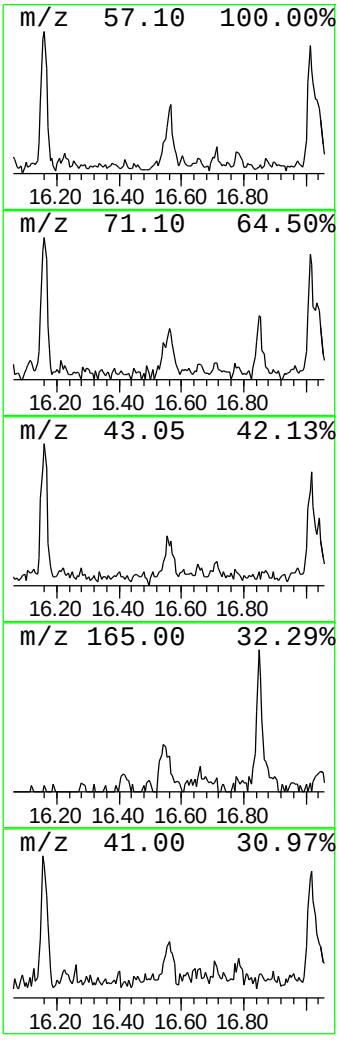
Peak Number 5 unknown16.56 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.56	2.30 ng	51596	Acenaphthene-d10	15.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	30
2	Heptadecane, 7-methyl-	254	C18H38	020959-33-5	27
3	Sulfurous acid, dodecyl 2-ethylh...	362	C20H42O3S	1000309-19-5	27
4	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	25
5	Decane, 1-bromo-2-methyl-	234	C11H23Br	127839-47-8	22





Data Path : Z:\HPCHEM1\BNA G\DATA\BG011918\
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Operator : SJ/JU
Sample : J1205-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.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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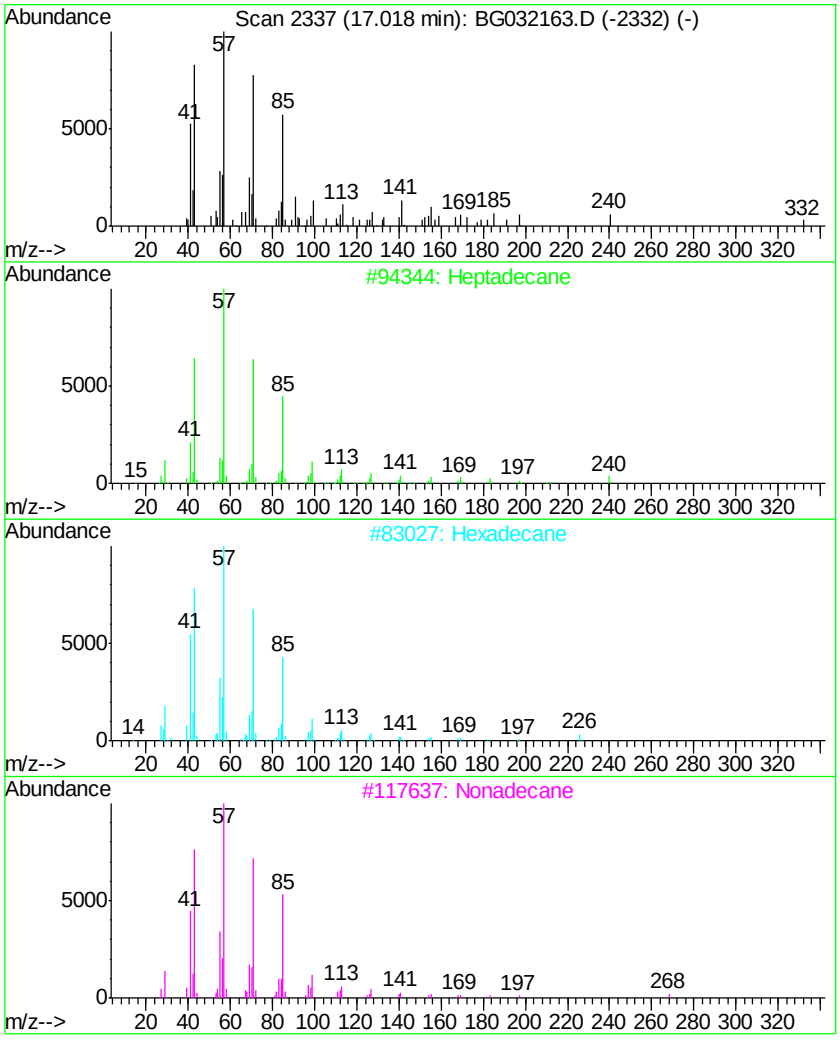
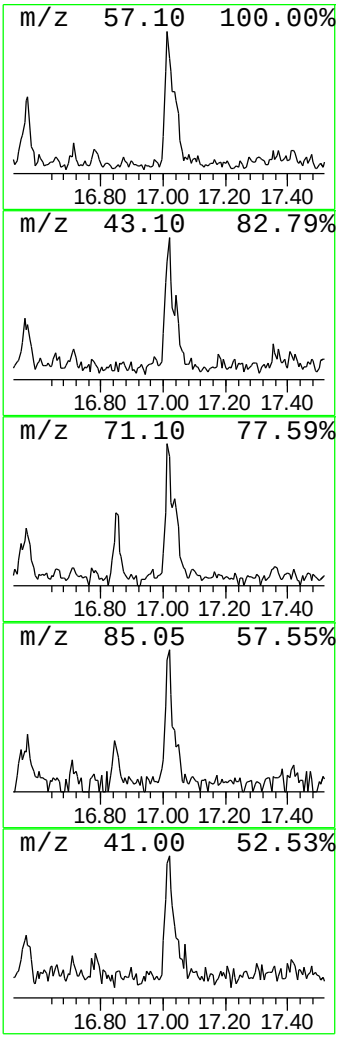
Peak Number 6 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.02	2.58 ng	87609	Phenanthrene-d10	18.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	90
2	Hexadecane	226	C16H34	000544-76-3	83
3	Nonadecane	268	C19H40	000629-92-5	83
4	Decane, 2,3,7-trimethyl-	184	C13H28	062238-13-5	80
5	Octadecane	254	C18H38	000593-45-3	80





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Misc :
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Instrument : BNA_G
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.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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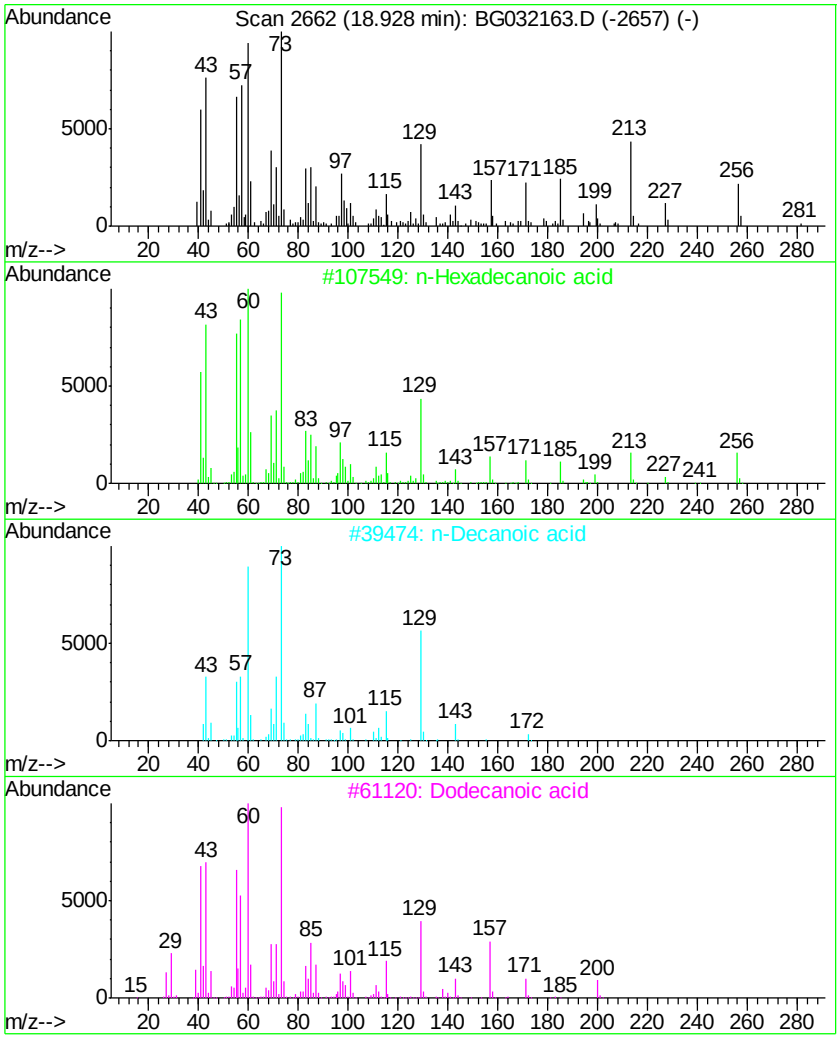
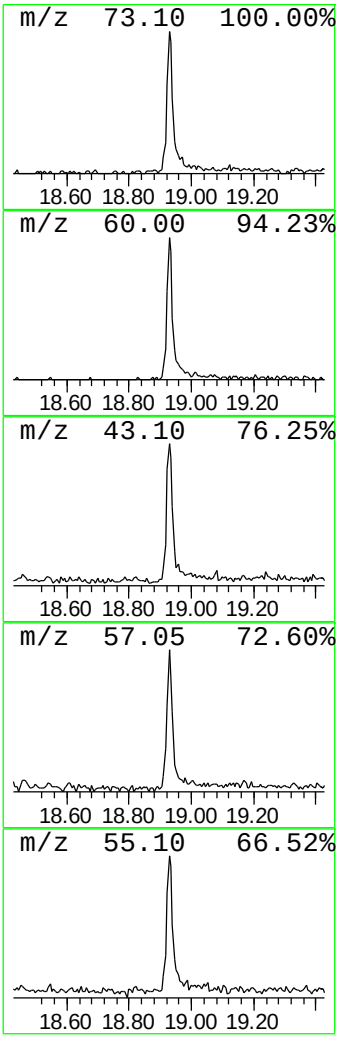
Peak Number 7 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.93	6.59 ng	224018	Phenanthrene-d10	18.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	n-Decanoic acid	172	C10H20O2	000334-48-5	89
3	Dodecanoic acid	200	C12H24O2	000143-07-7	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5	Tridecanoic acid	214	C13H26O2	000638-53-9	52





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Instrument : BNA_G
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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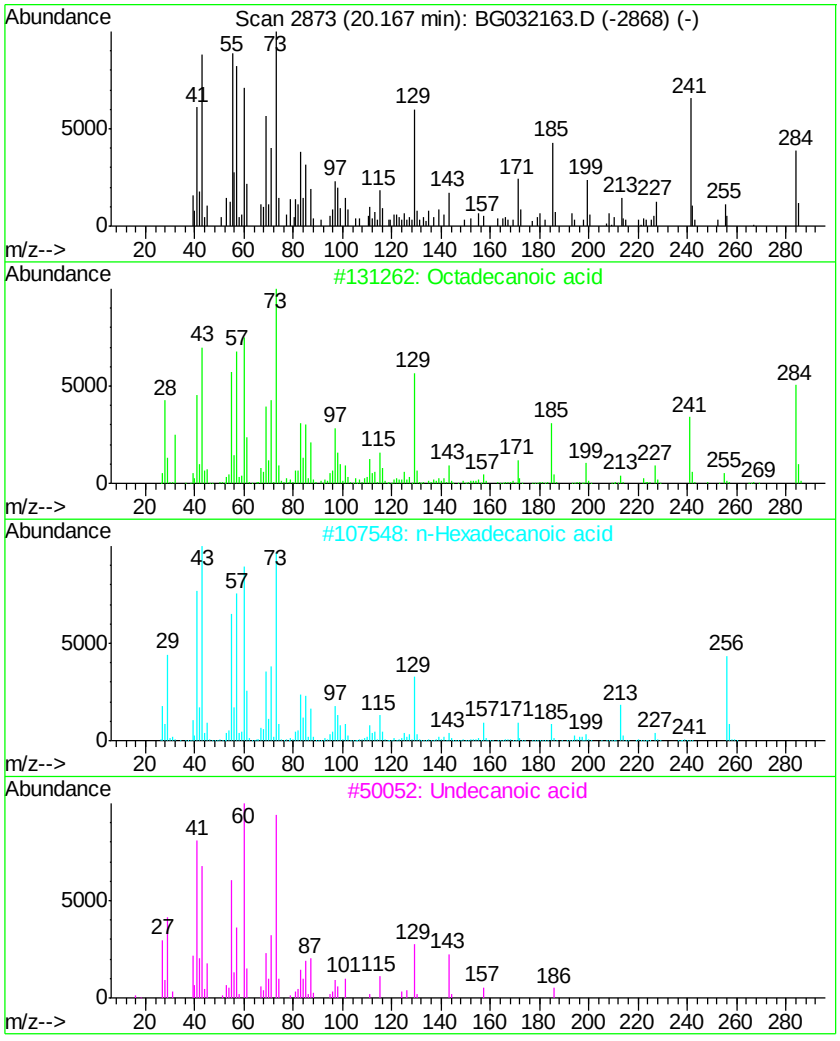
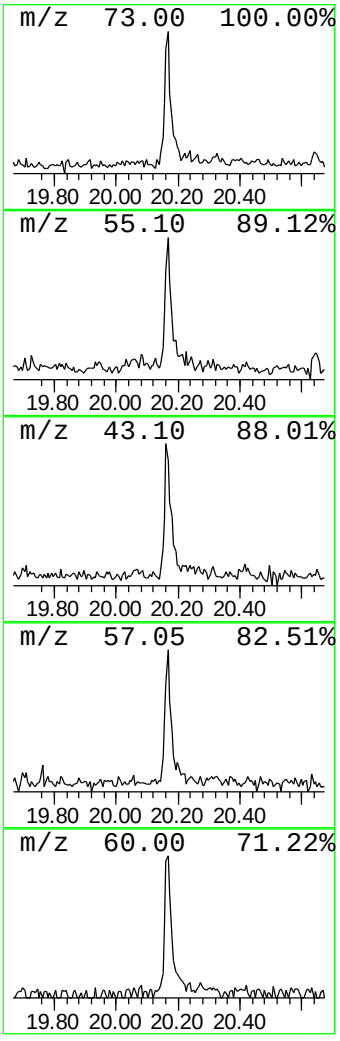
Peak Number 8 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.17	3.72 ng	126554	Phenanthrene-d10	18.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	59
3	Undecanoic acid	186	C11H22O2	000112-37-8	53
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	43
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	38





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Instrument : BNA_G
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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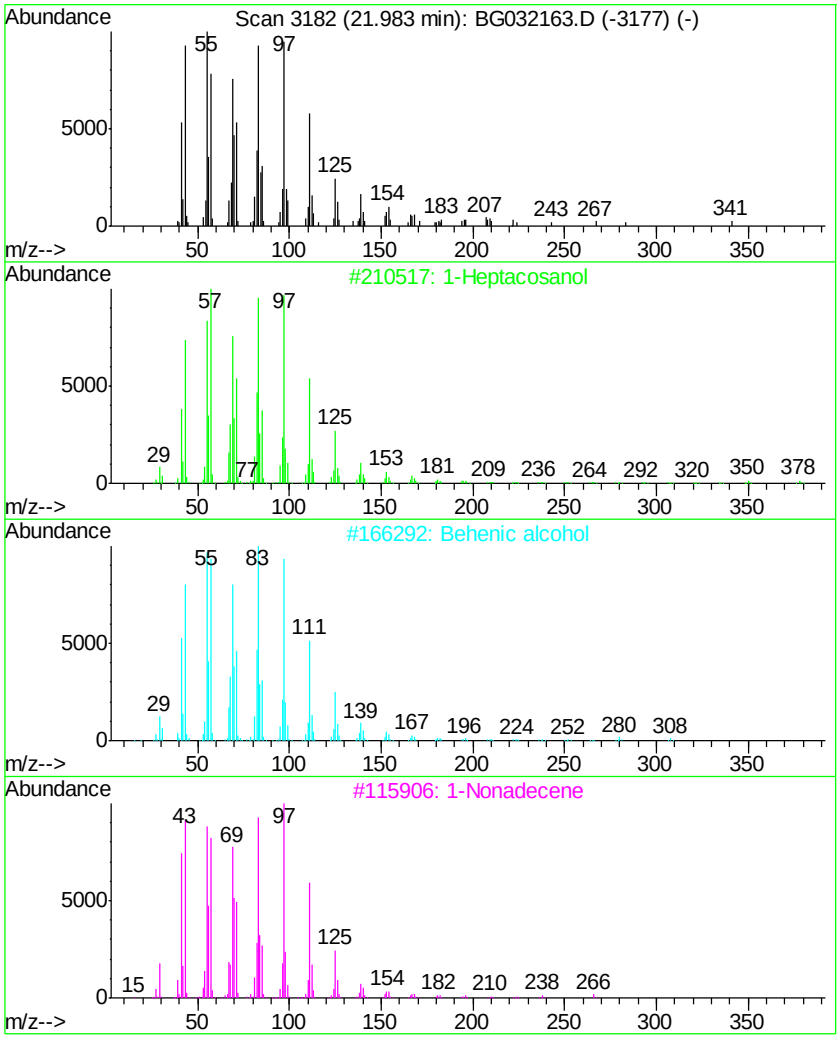
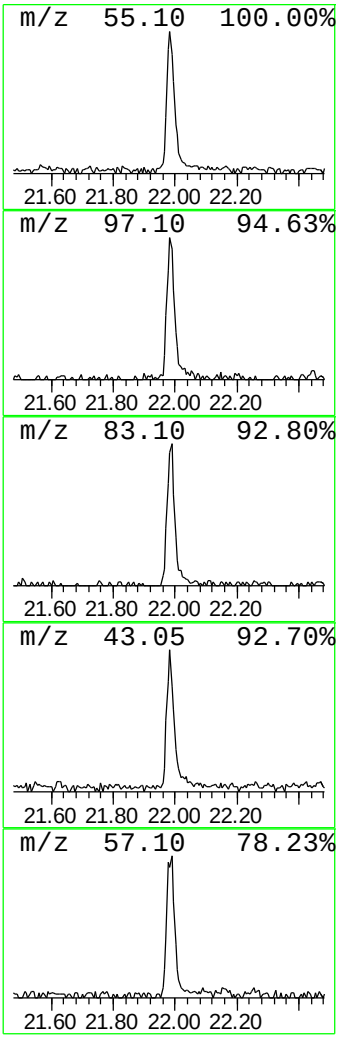
Peak Number 9 1-Heptacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.98	3.31 ng	168722	Chrysene-d12	22.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	95
2	Behenic alcohol	326	C22H46O	000661-19-8	94
3	1-Nonadecene	266	C19H38	018435-45-5	91
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91





Tentatively Identified Compound (LSC) summary

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
5-Aminoindole	8.25	53.1	ng	568802	1	8.75	214194	20.0
Sulfurous acid, 2...	15.22	2.0	ng	46028	3	15.37	448487	20.0
Hexadecane	16.16	3.1	ng	70691	3	15.37	448487	20.0
unknown16.56	16.56	2.3	ng	51596	3	15.37	448487	20.0
Heptadecane	17.02	2.6	ng	87609	4	18.11	680299	20.0
n-Hexadecanoic acid	18.93	6.6	ng	224018	4	18.11	680299	20.0
Octadecanoic acid	20.17	3.7	ng	126554	4	18.11	680299	20.0
1-Heptacosanol	21.98	3.3	ng	168722	5	22.45	1019050	20.0