LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061918\
Data File : BG035254.D
Acq On : 19 Jun 2018 19:00
Operator : SJ/JU
Sample : J3546-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 061418-DBRC-F-U-B

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-BG060718.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	5.629	392	398	410	rBV	161667	293266	4.99%	1.856%
2	7.215	661	668	678	rBV	121600	224575	3.82%	1.422%
3	7.591	724	732	742	rVB	303224	530180	9.02%	3.356%
4	8.061	806	812	820	rBV	92039	151419	2.58%	0.958%
5	8.384	858	867	876	rVB	402403	710986	12.10%	4.500%
6	9.219	1002	1009	1022	rBV	350190	639094	10.88%	4.045%
7	10.863	1282	1289	1301	rBV	112895	207216	3.53%	1.312%
8	13.307	1697	1705	1715	rBV	1046797	1616324	27.51%	10.231%
9	14.130	1839	1845	1851	rBV	45548	68638	1.17%	0.434%
10	14.682	1931	1939	1948	rBV3	216322	356706	6.07%	2.258%
11	16.033	2163	2169	2175	rVB	43398	67215	1.14%	0.425%
12	16.162	2184	2191	2201	rBV	798915	1192931	20.30%	7.551%
13	17.425	2400	2406	2413	rBV	427653	626788	10.67%	3.967%
14	18.306	2551	2556	2572	rBV2	133663	208602	3.55%	1.320%
15	19.575	2767	2772	2781	rBV2	115736	160247	2.73%	1.014%
16	20.033	2843	2850	2863	rBV	4413278	5875643	100.00%	37.192%
17	21.690	3125	3132	3140	rBV2	710755	1199684	20.42%	7.594%
18	22.501	3262	3270	3274	rBV2	41046	72057	1.23%	0.456%
19	23.194	3383	3388	3397	rVB2	69323	122679	2.09%	0.777%
20	24.004	3518	3526	3534	rVB2	83088	171980	2.93%	1.089%
21	24.921	3670	3682	3696	rBV3	341001	1152611	19.62%	7.296%
22	26.090	3874	3881	3892	rVB4	53930	149270	2.54%	0.945%

Sum of corrected areas: 15798111

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061918\
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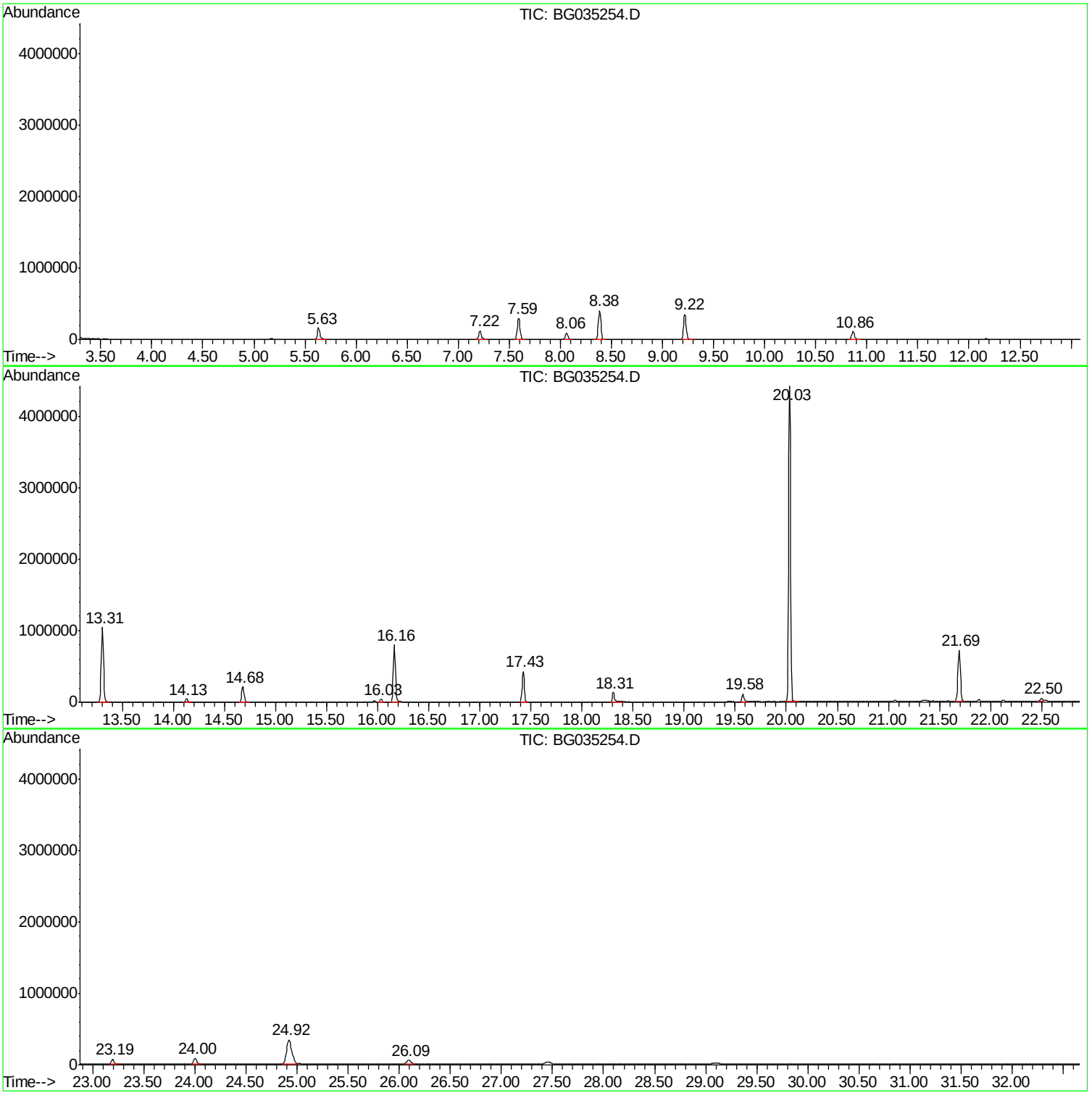
Sample : J3546-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
061418-DBRC-F-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061918\
Data File : BG035254.D
Acq On : 19 Jun 2018 19:00
Operator : SJ/JU
Sample : J3546-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 061418-DBRC-F-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.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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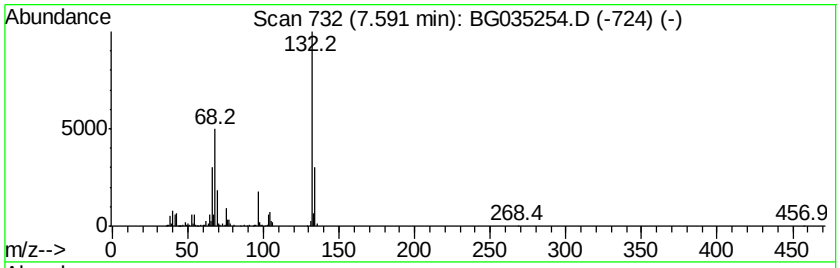
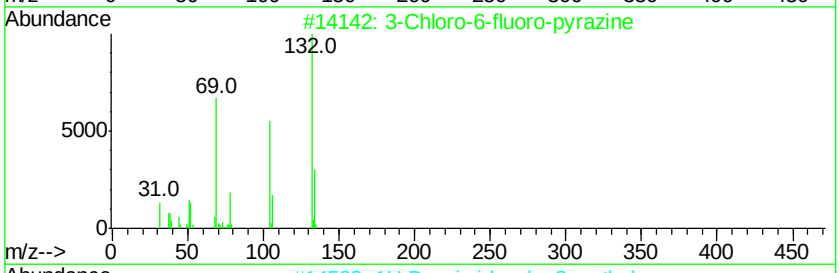
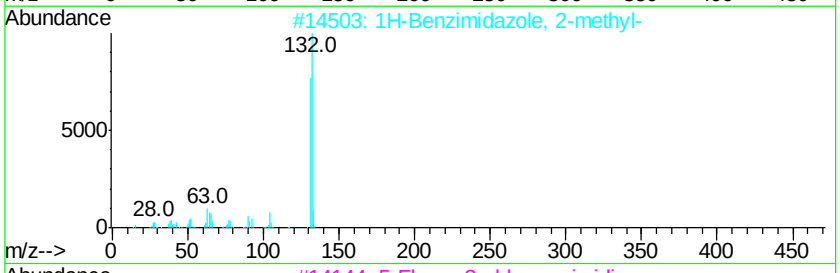
Peak Number 1 unknown7.59 Concentration Rank 2

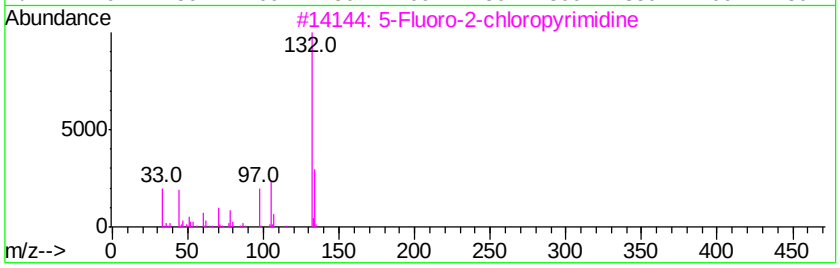
R.T.	EstConc	Area	Relative to ISTD	R.T.
7.59	70.03 ng	530180	1,4-Dichlorobenzene-d4	8.06

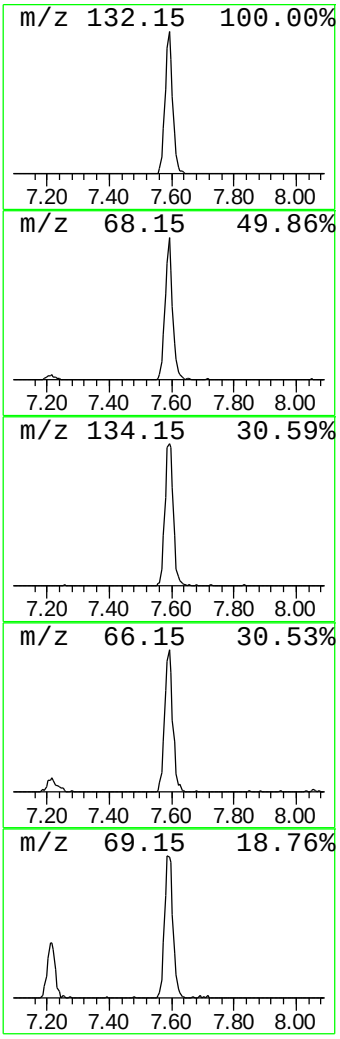
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1H-Indazole, 3-methyl-	132	C8H8N2	1000316-00-2	10











Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061918\
Data File : BG035254.D
Acq On : 19 Jun 2018 19:00
Operator : SJ/JU
Sample : J3546-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 061418-DBRC-F-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.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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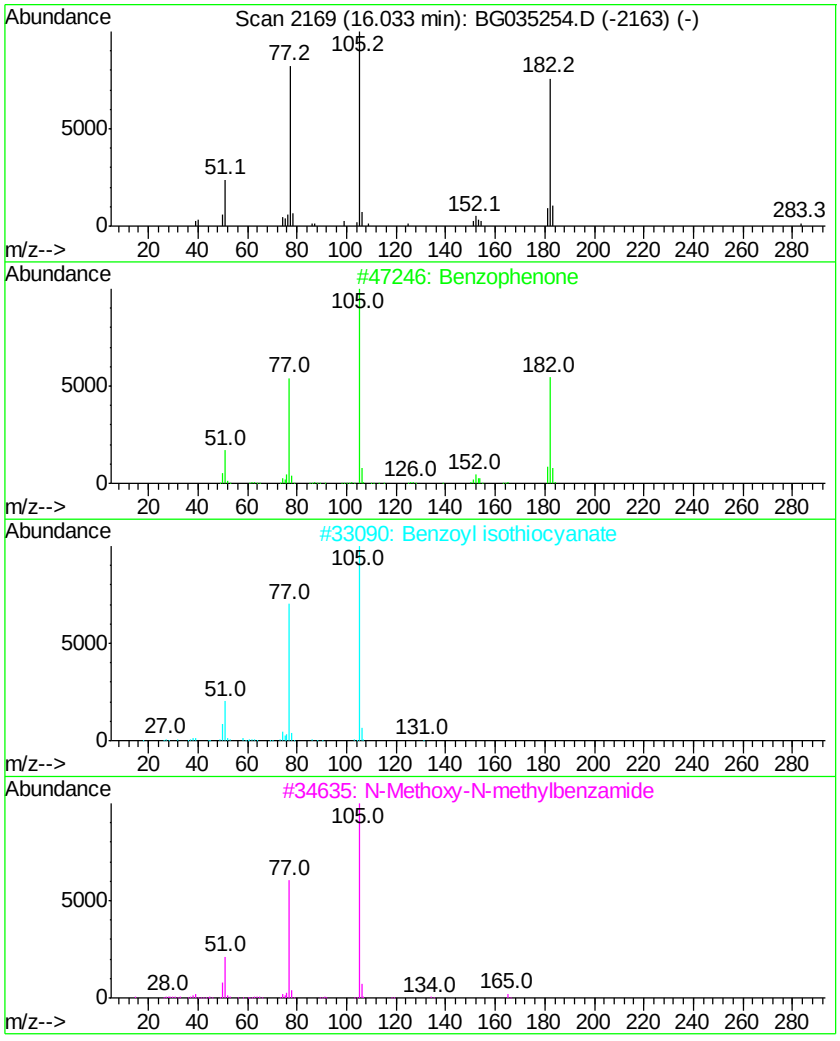
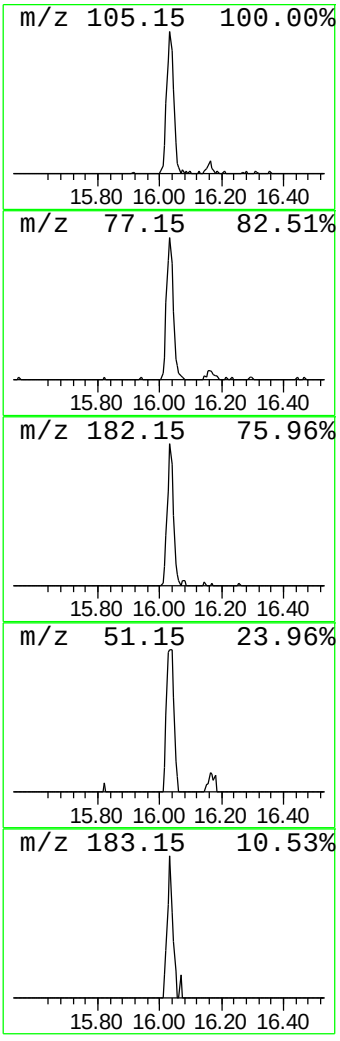
Peak Number 3 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.03	3.77 ng	67215	Acenaphthene-d10	14.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	94
2	Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	43
3	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	43
4	Benzoyl bromide	184	C7H5BrO	000618-32-6	43
5	2-Phenyl-4-ethylidene-2-oxazolin...	187	C11H9NO2	037791-41-6	43





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061918\
Data File : BG035254.D
Acq On : 19 Jun 2018 19:00
Operator : SJ/JU
Sample : J3546-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 061418-DBRC-F-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.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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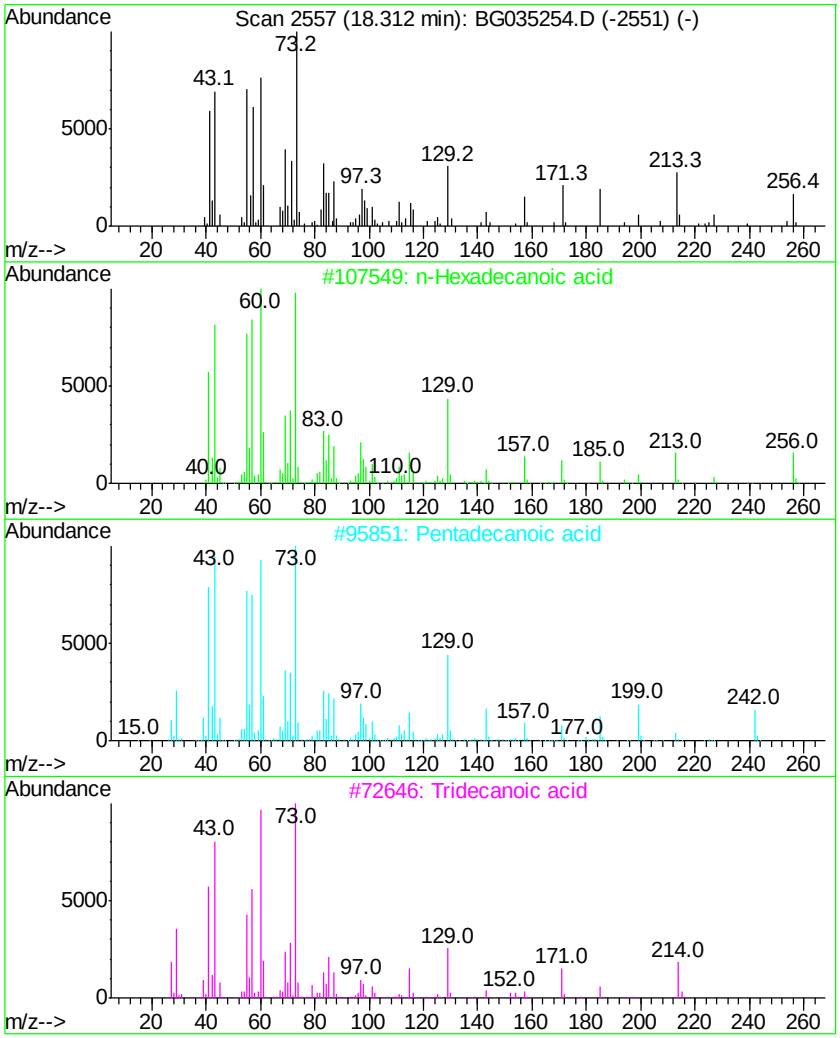
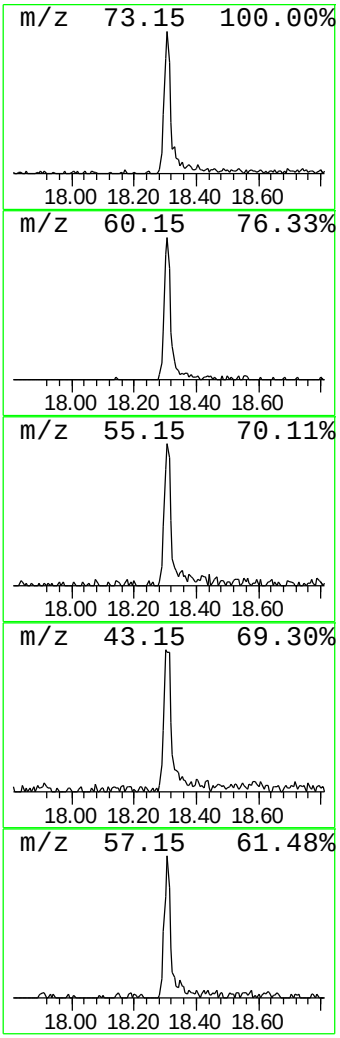
Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.31	6.66 ng	208602	Phenanthrene-d10	17.43

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	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	64
4	n-Decanoic acid	172	C10H20O2	000334-48-5	58
5	i-Propyl 14-methyl-pentadecanoate	298	C19H38O2	1000336-62-4	50





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061918\
Data File : BG035254.D
Acq On : 19 Jun 2018 19:00
Operator : SJ/JU
Sample : J3546-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 061418-DBRC-F-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.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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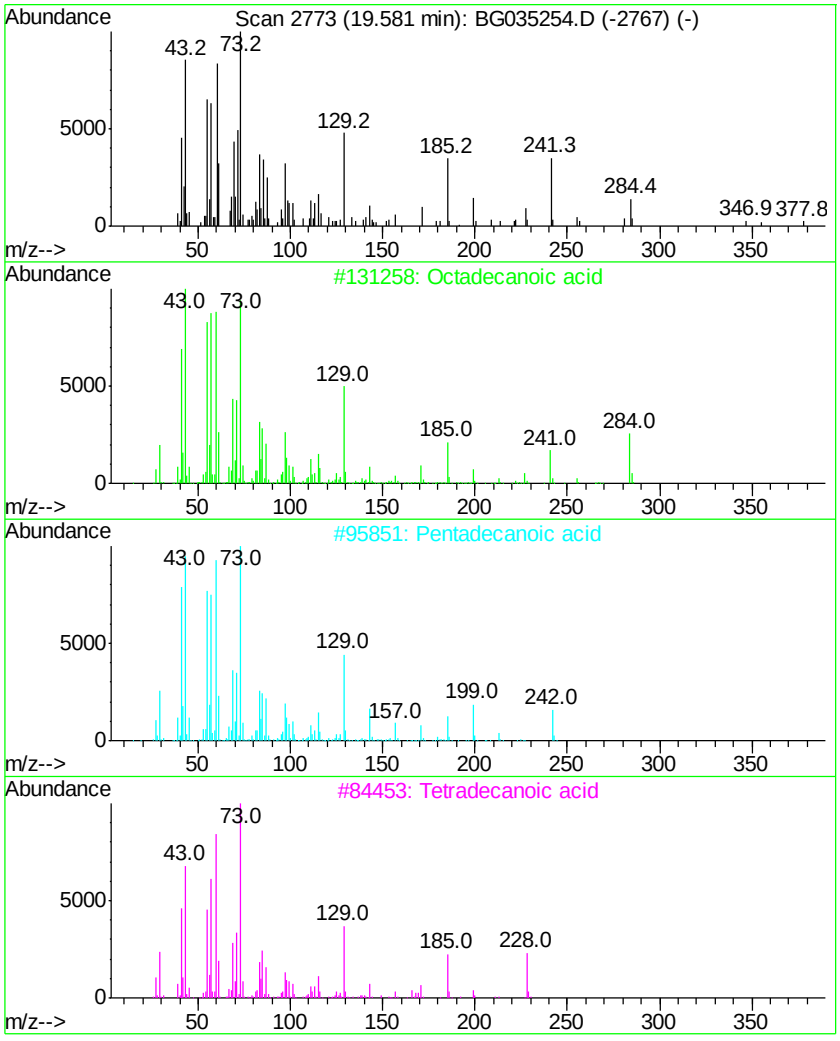
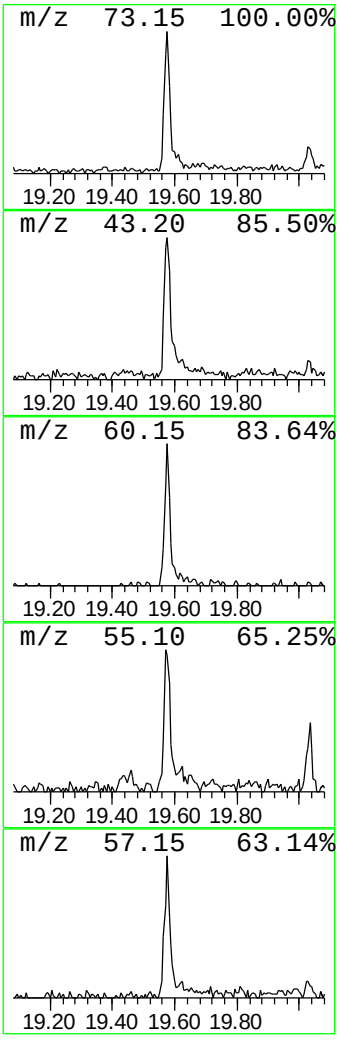
Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.58	2.67 ng	160247	Chrysene-d12	21.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Dodecanoic acid	200	C12H24O2	000143-07-7	58
5	Tridecanoic acid	214	C13H26O2	000638-53-9	53





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061918\
Data File : BG035254.D
Acq On : 19 Jun 2018 19:00
Operator : SJ/JU
Sample : J3546-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 061418-DBRC-F-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.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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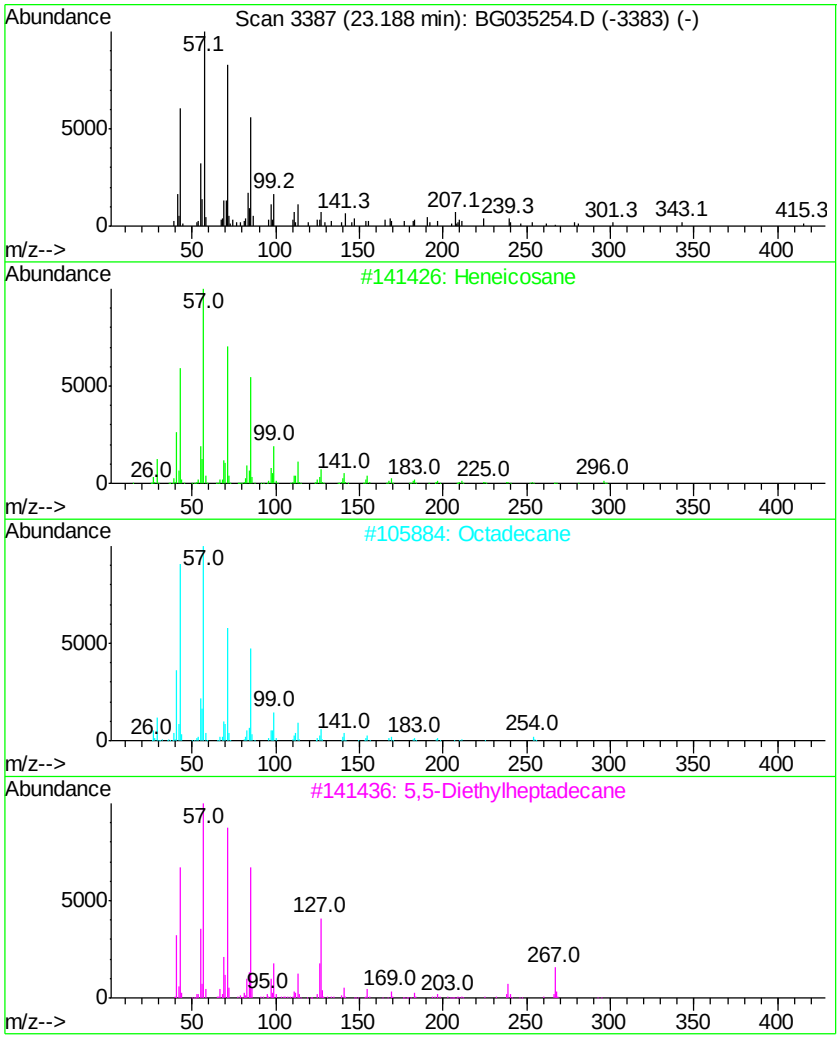
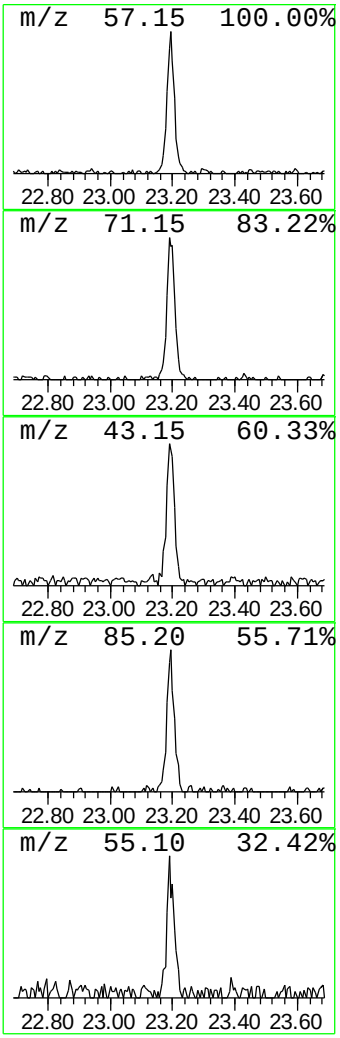
Peak Number 6 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.19	2.05 ng	122679	Chrysene-d12	21.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	87
2	Octadecane	254	C18H38	000593-45-3	86
3	5,5-Diethylheptadecane	296	C21H44	1000360-41-7	86
4	6,6-Diethylhoctadecane	310	C22H46	1000360-41-8	86
5	10-Methylnonadecane	282	C20H42	056862-62-5	86





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061918\
Data File : BG035254.D
Acq On : 19 Jun 2018 19:00
Operator : SJ/JU
Sample : J3546-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 061418-DBRC-F-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.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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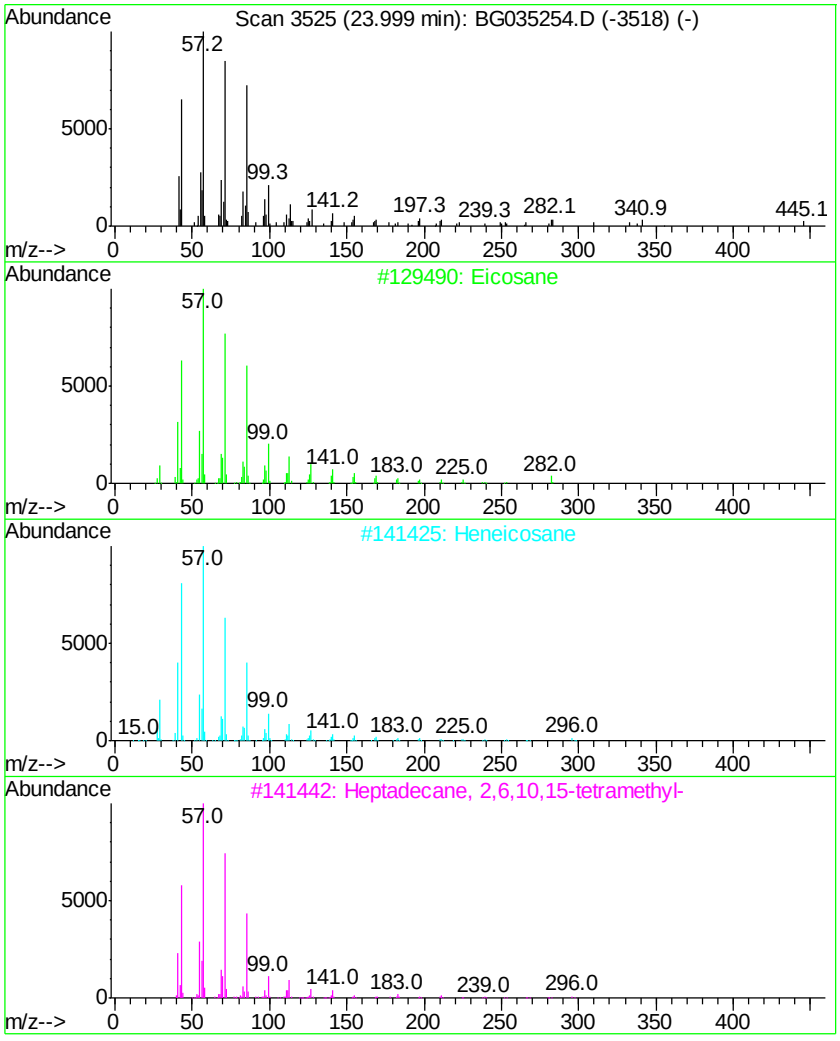
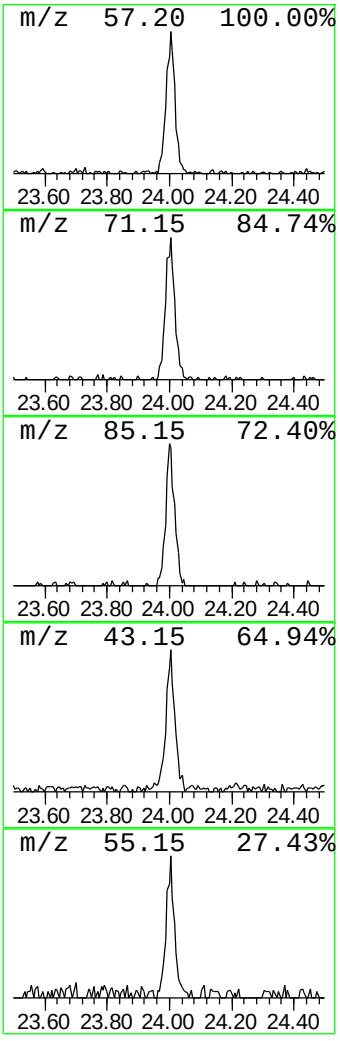
Peak Number 7 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.00	2.98 ng	171980	Perylene-d12	24.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Heneicosane	296	C21H44	000629-94-7	94
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91
4	Hexacosane	366	C26H54	000630-01-3	91
5	Triacontane	422	C30H62	000638-68-6	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061918\
Data File : BG035254.D
Acq On : 19 Jun 2018 19:00
Operator : SJ/JU
Sample : J3546-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 061418-DBRC-F-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.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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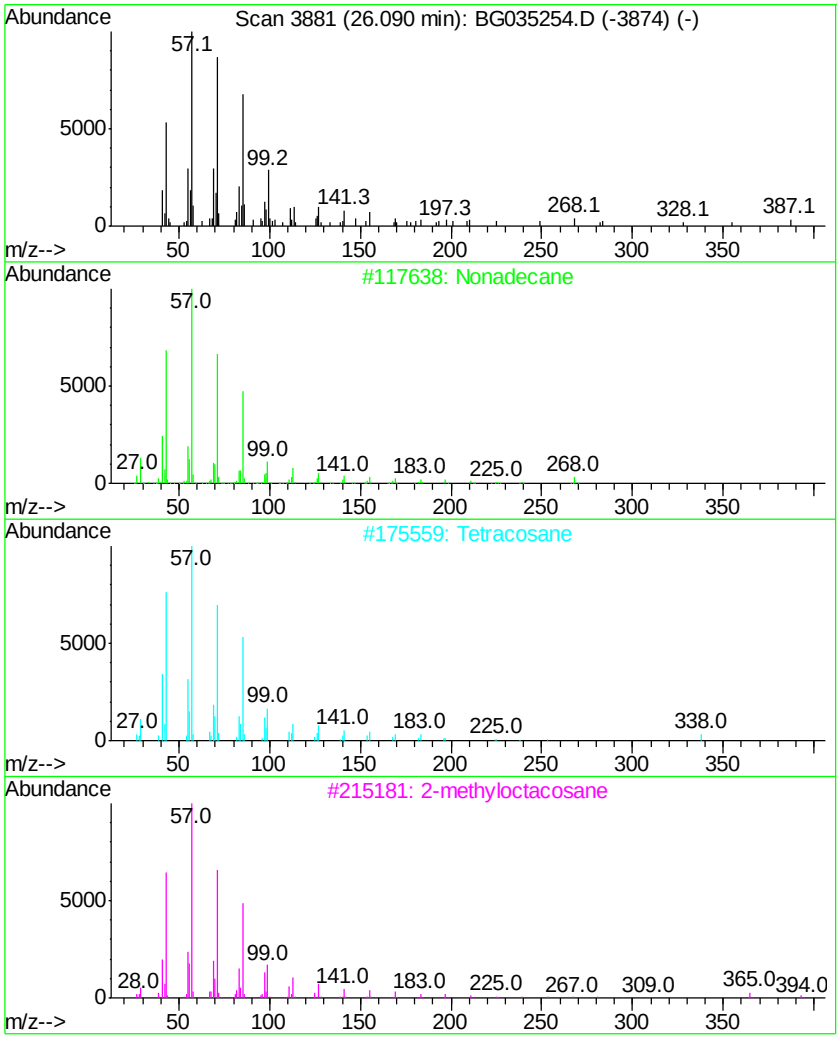
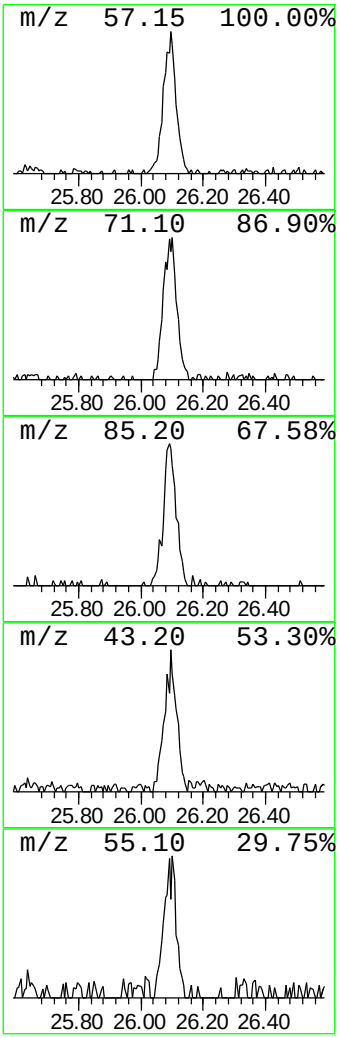
Peak Number 8 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.09	2.59 ng	149270	Perylene-d12	24.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	90
2	Tetracosane	338	C24H50	000646-31-1	83
3	2-methyloctacosane	408	C29H60	1000376-72-8	83
4	Hexacosane	366	C26H54	000630-01-3	83
5	Heneicosane	296	C21H44	000629-94-7	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG061918\
Data File : BG035254.D
Acq On : 19 Jun 2018 19:00
Operator : SJ/JU
Sample : J3546-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 061418-DBRC-F-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.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
unknown7.59	7.59	70.0	ng	530180	1	8.06	151419	20.0
Benzophenone	16.03	3.8	ng	67215	3	14.68	356706	20.0
n-Hexadecanoic acid	18.31	6.7	ng	208602	4	17.43	626788	20.0
Octadecanoic acid	19.58	2.7	ng	160247	5	21.69	1199680	20.0
Heneicosane	23.19	2.0	ng	122679	5	21.69	1199680	20.0
Eicosane	24.00	3.0	ng	171980	6	24.92	1152610	20.0
Nonadecane	26.09	2.6	ng	149270	6	24.92	1152610	20.0