LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG100419\
Data File : BG043032.D
Acq On : 4 Oct 2019 17:39
Operator : JU
Sample : PB123594BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB123594BL

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-BG092519.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	3.173	6	14	22	rBV2	51454	127673	2.17%	0.456%
2	3.255	22	28	39	rVB	67515	125890	2.14%	0.450%
3	5.646	428	435	447	rBV	1116874	1808398	30.74%	6.460%
4	7.233	695	705	718	rBV	1170613	2046475	34.78%	7.310%
5	7.603	759	768	777	rBV	1121965	1985592	33.75%	7.093%
6	8.061	839	846	854	rBV	242894	420855	7.15%	1.503%
7	8.384	893	901	911	rBV	865533	1567514	26.64%	5.599%
8	9.219	1034	1043	1054	rBV	653159	1229306	20.89%	4.391%
9	10.864	1316	1323	1332	rBV	291206	534281	9.08%	1.908%
10	13.308	1731	1739	1751	rBV	2022085	3134769	53.28%	11.197%
11	14.131	1872	1879	1884	rBV2	102053	157854	2.68%	0.564%
12	14.683	1966	1973	1982	rBV	498007	796122	13.53%	2.844%
13	16.169	2217	2226	2236	rBV	1876696	2944609	50.05%	10.518%
14	17.421	2433	2439	2451	rBV2	652700	1034173	17.58%	3.694%
15	20.035	2877	2884	2893	rBV	4335621	5883675	100.00%	21.017%
16	21.346	3102	3107	3113	rBV3	62331	147193	2.50%	0.526%
17	21.692	3159	3166	3178	rBV2	750143	1288636	21.90%	4.603%
18	21.886	3195	3199	3205	rVB3	41559	60643	1.03%	0.217%
19	22.497	3298	3303	3309	rBV2	55355	92645	1.57%	0.331%
20	23.191	3415	3421	3428	rVB2	105444	209936	3.57%	0.750%
21	23.995	3552	3558	3569	rVB3	131921	299268	5.09%	1.069%
22	24.912	3703	3714	3730	rVB3	470569	1672167	28.42%	5.973%
23	26.081	3905	3913	3924	rVB	102700	283249	4.81%	1.012%
24	27.438	4139	4144	4156	rVB7	48957	144367	2.45%	0.516%

Sum of corrected areas: 27995290

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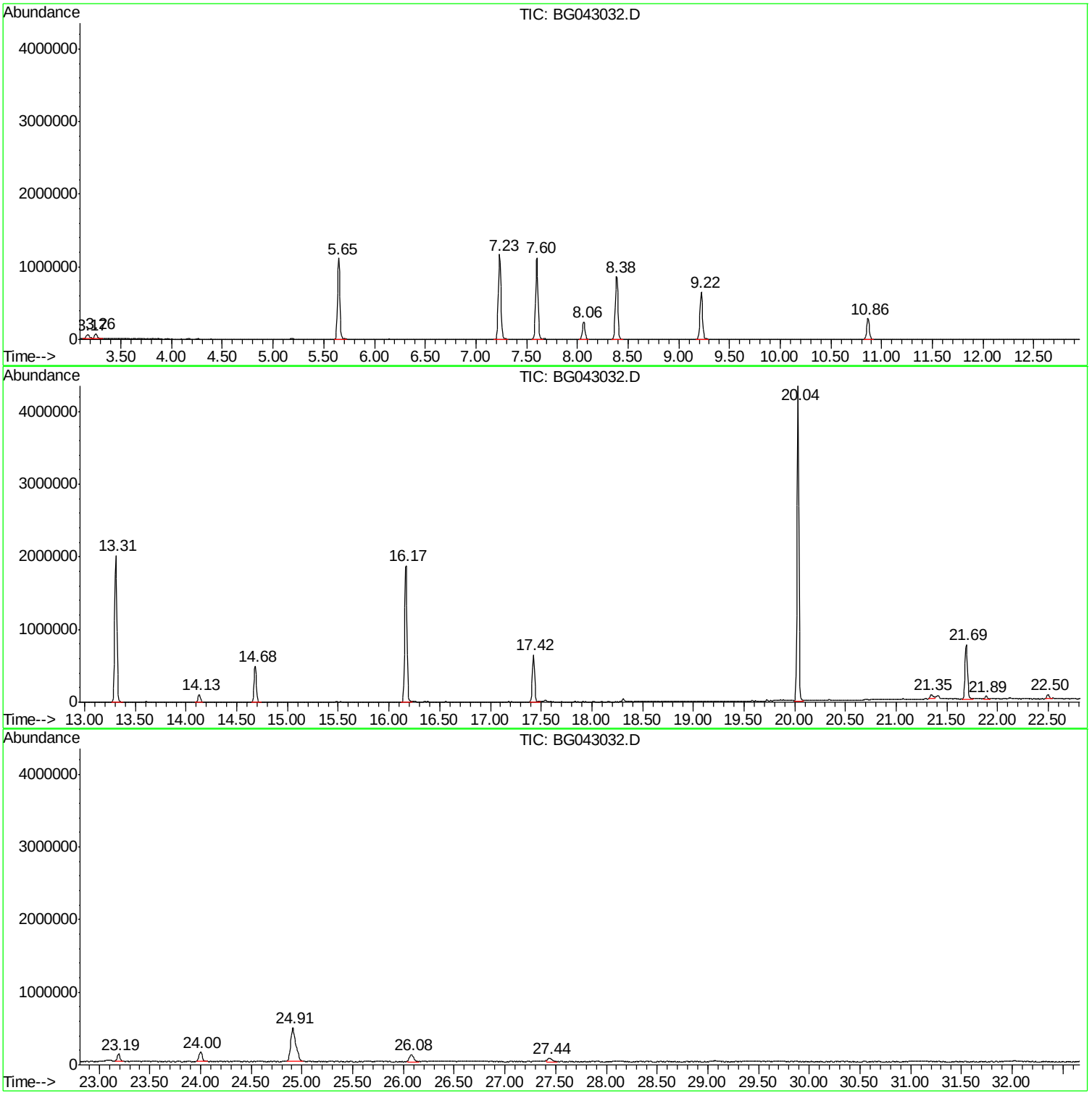
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB123594BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG100419\
Data File : BG043032.D
Acq On : 4 Oct 2019 17:39
Operator : JU
Sample : PB123594BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB123594BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.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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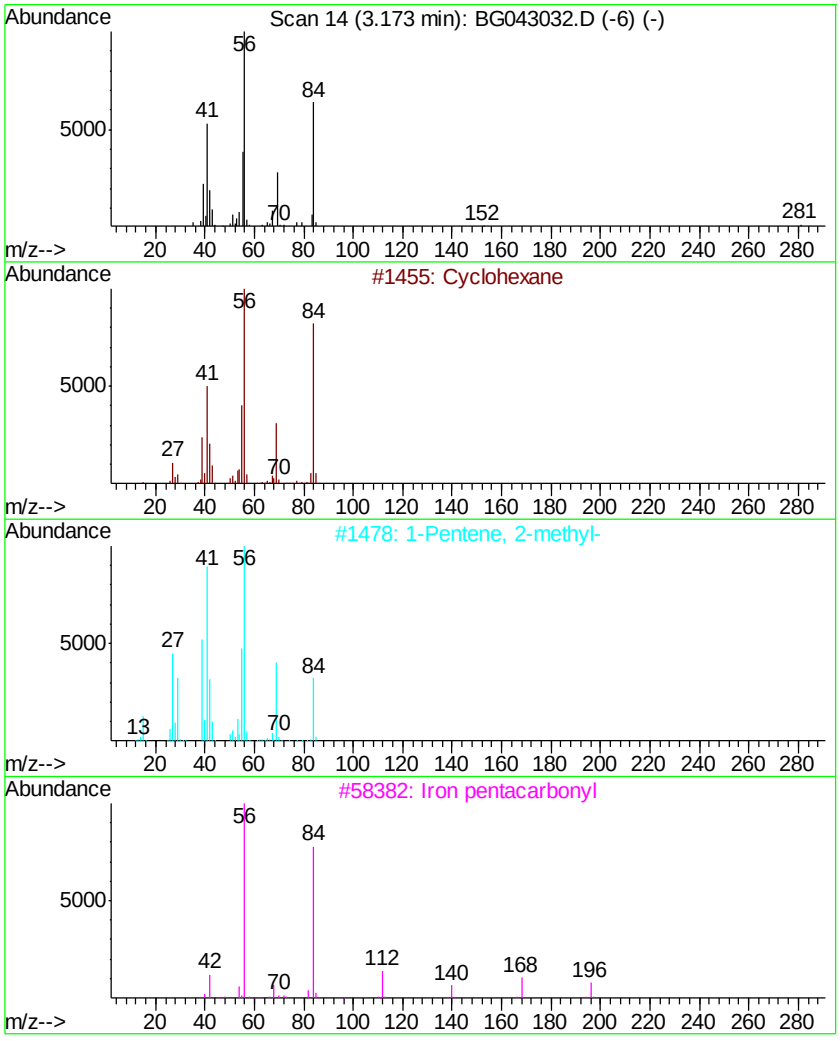
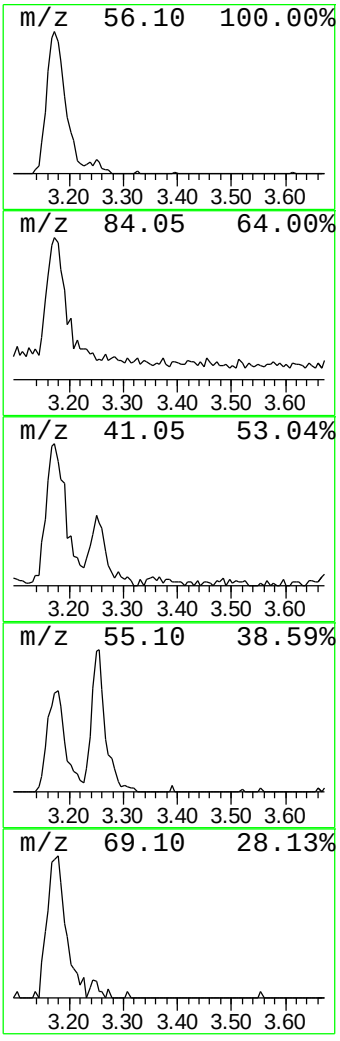
Peak Number 1 1-Pentene, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.17	6.07 ng	127673	1,4-Dichlorobenzene-d4	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane	84	C6H12	000110-82-7	90
2	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	78
3	Iron pentacarbonyl	196	C5FeO5	013463-40-6	56
4	Cyclobutane	56	C4H8	000287-23-0	43
5	2-Amino-oxazole	84	C3H4N2O	004570-45-0	43





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG100419\
Data File : BG043032.D
Acq On : 4 Oct 2019 17:39
Operator : JU
Sample : PB123594BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB123594BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.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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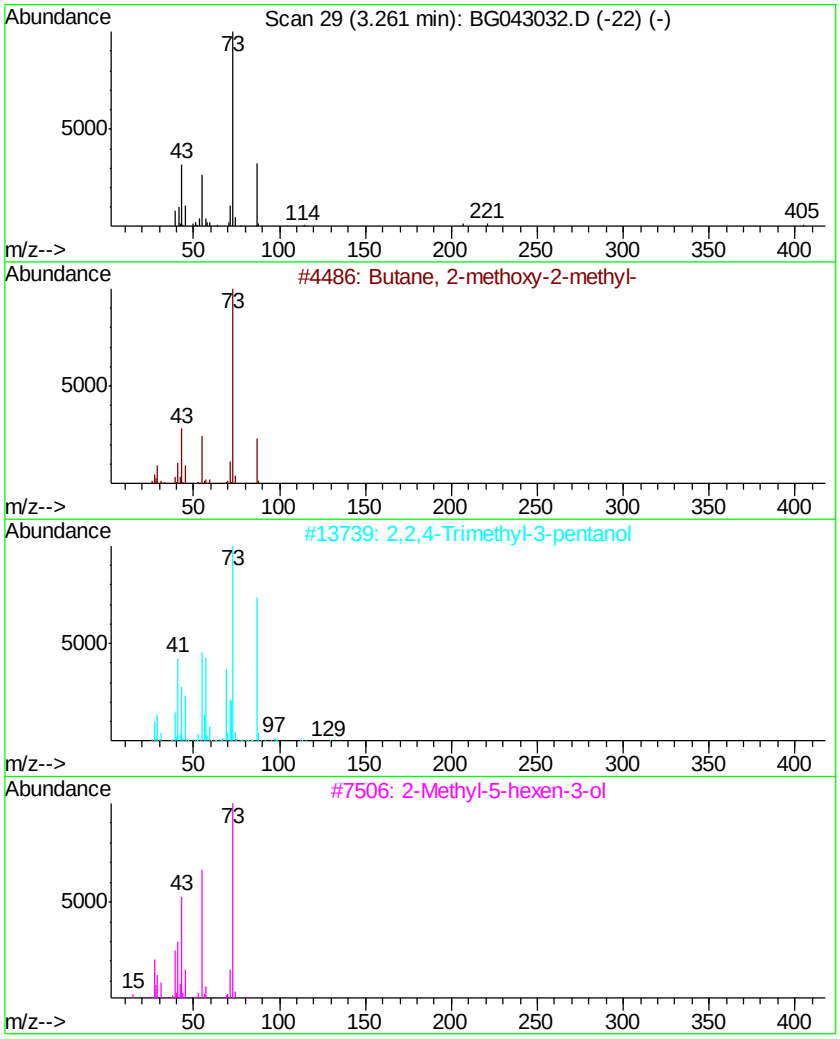
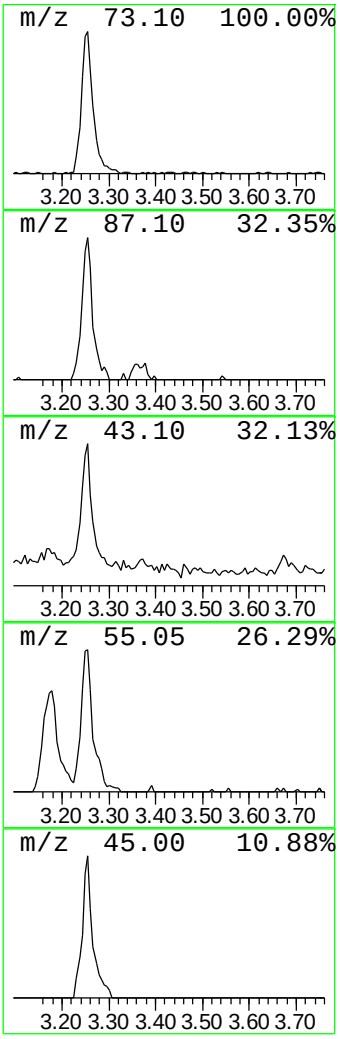
Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.26	5.98 ng	125890	1,4-Dichlorobenzene-d4	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5	1,3-Dioxolane, 2-heptyl-	172	C10H20O2	004359-57-3	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG100419\
Data File : BG043032.D
Acq On : 4 Oct 2019 17:39
Operator : JU
Sample : PB123594BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB123594BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

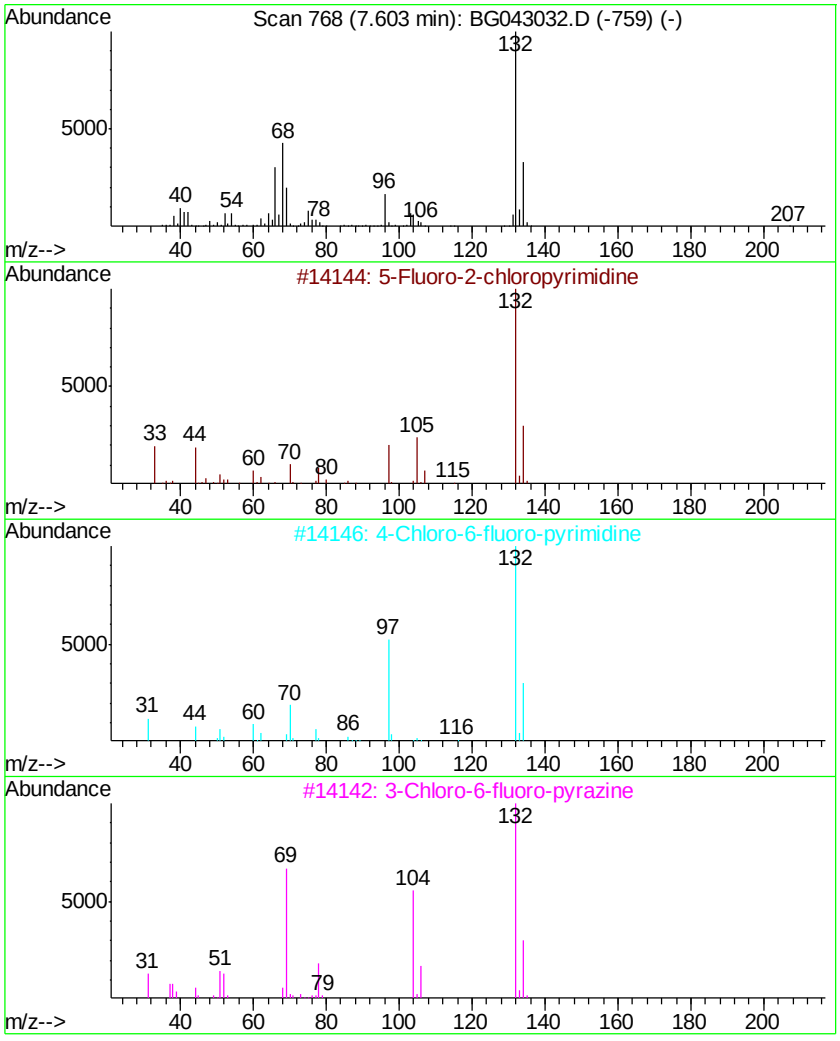
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

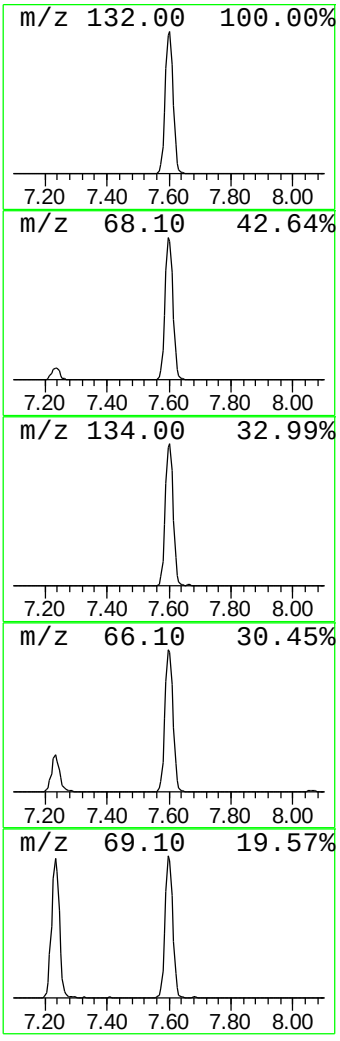
****

Peak Number 3 unknown7.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.60	94.36 ng	1985590	1,4-Dichlorobenzene-d4	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
4	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	22
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22





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Data File : BG043032.D
Acq On : 4 Oct 2019 17:39
Operator : JU
Sample : PB123594BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB123594BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

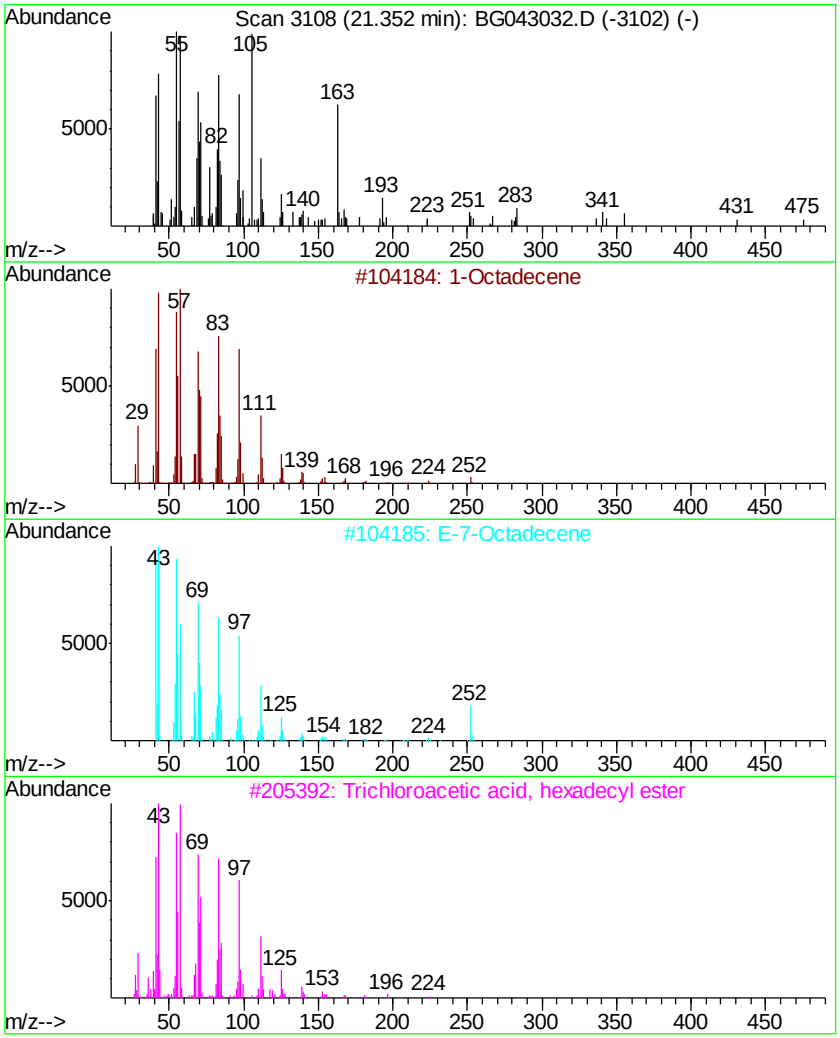
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

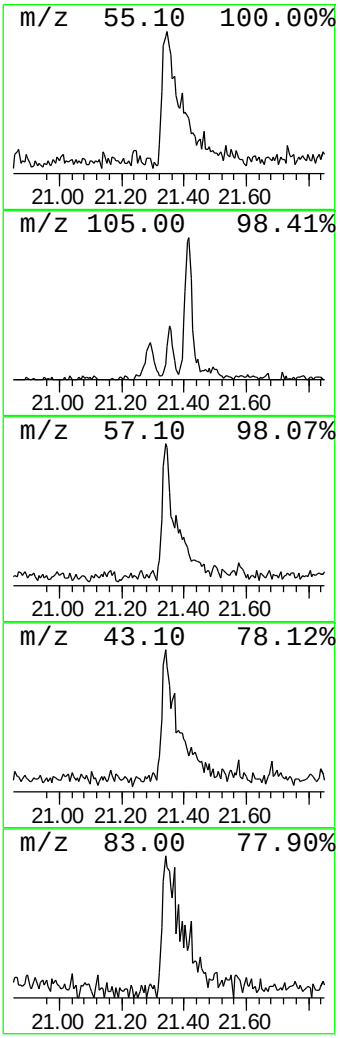
****

Peak Number 5 1-Octadecene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.35	2.28 ng	147193	Chrysene-d12	21.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene	252	C18H36	000112-88-9	90
2	E-7-Octadecene	252	C18H36	1000130-92-0	83
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	81
4	E-15-Heptadecenal	252	C17H32O	1000130-97-9	78
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	68





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG100419\
Data File : BG043032.D
Acq On : 4 Oct 2019 17:39
Operator : JU
Sample : PB123594BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB123594BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

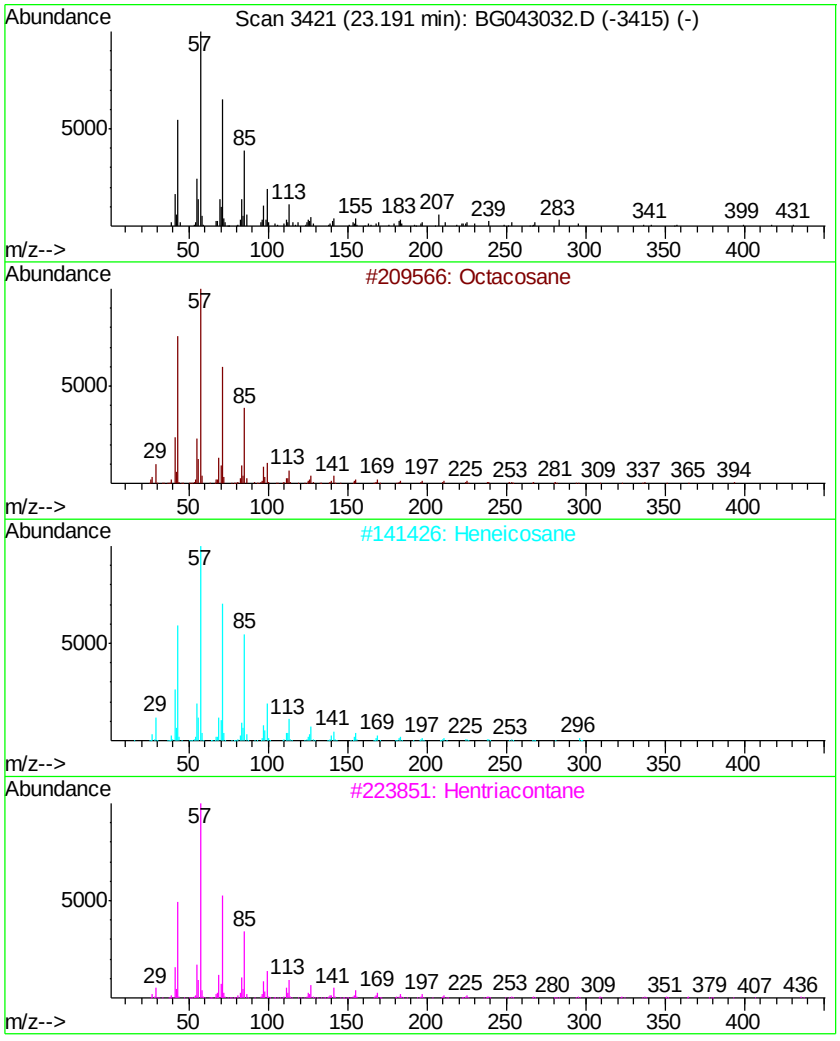
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

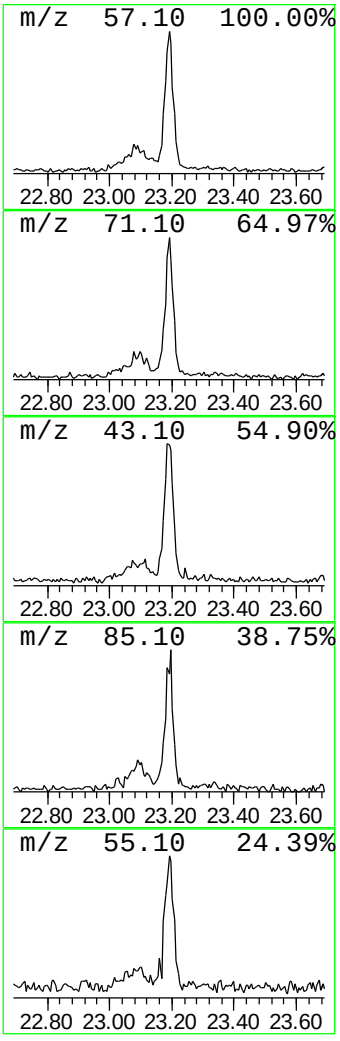
****

Peak Number 6 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.19	3.26 ng	209936	Chrysene-d12	21.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	87
2	Heneicosane	296	C21H44	000629-94-7	87
3	Hentriacontane	437	C31H64	000630-04-6	86
4	Docosane, 7-hexyl-	394	C28H58	055373-86-9	86
5	Tetratetracontane	619	C44H90	007098-22-8	83





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG100419\
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Operator : JU
Sample : PB123594BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB123594BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.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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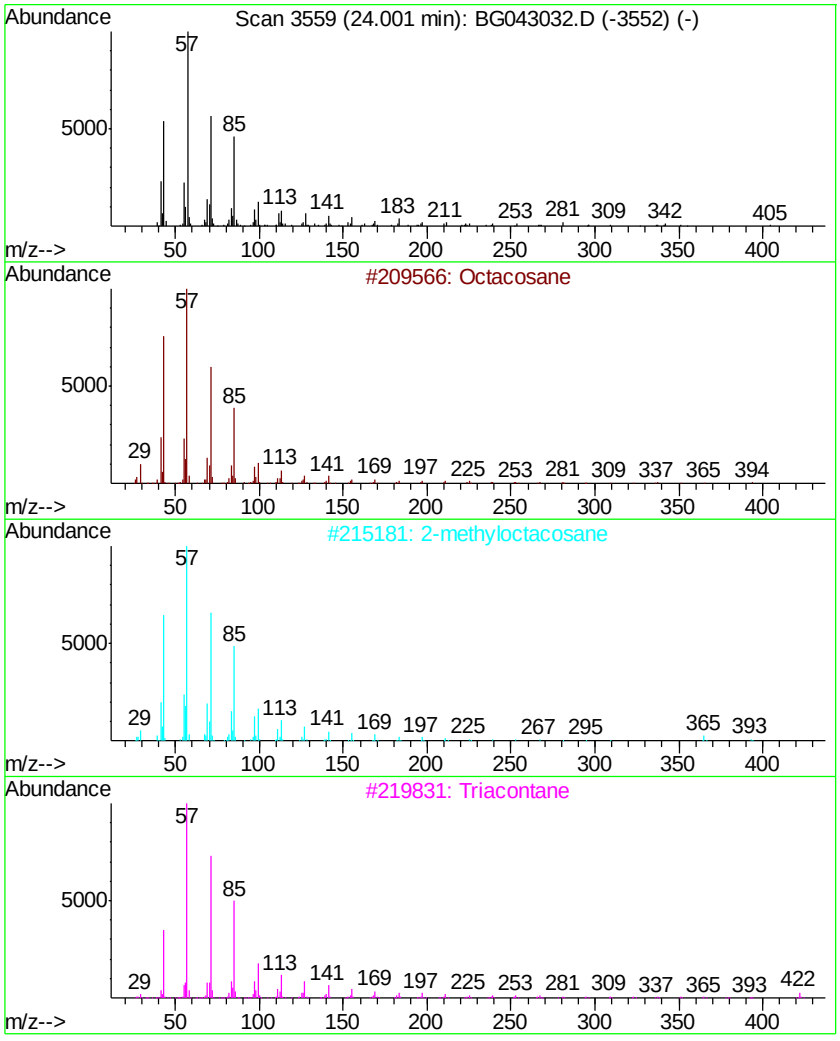
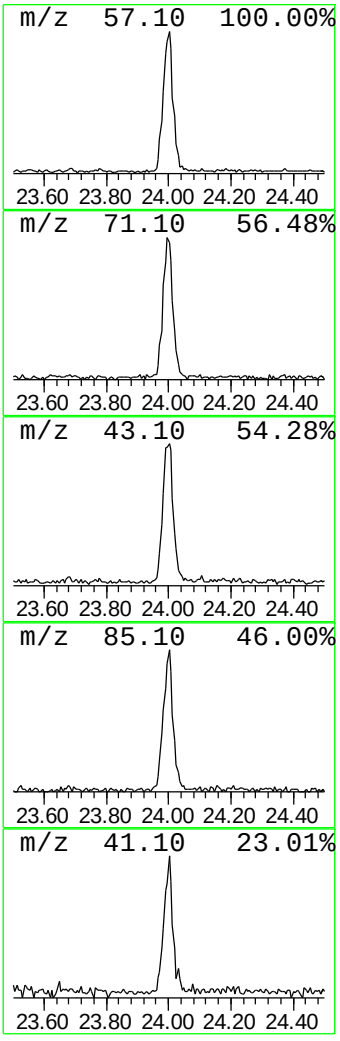
Peak Number 7 2-methyloctacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.00	3.58 ng	299268	Perylene-d12	24.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	87
2	2-methyloctacosane	408	C29H60	1000376-72-8	87
3	Triacontane	422	C30H62	000638-68-6	87
4	Tetratetracontane	619	C44H90	007098-22-8	87
5	Pentacosane	352	C25H52	000629-99-2	86





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Operator : JU
Sample : PB123594BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB123594BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.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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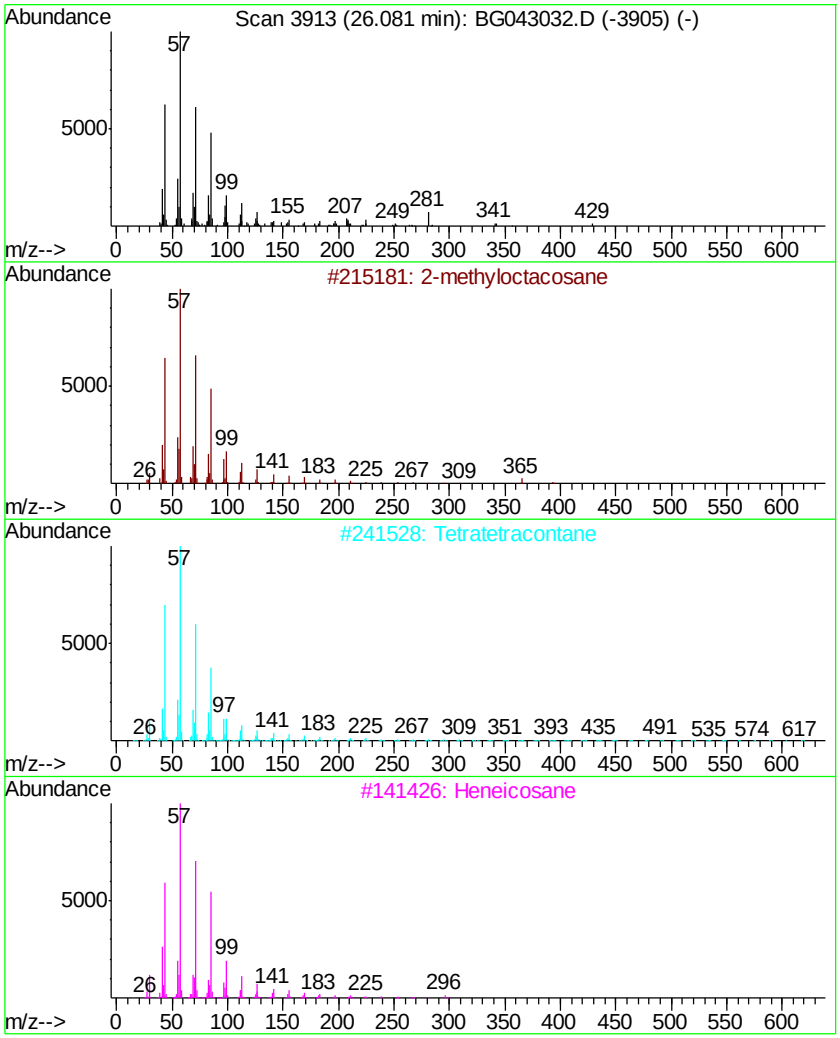
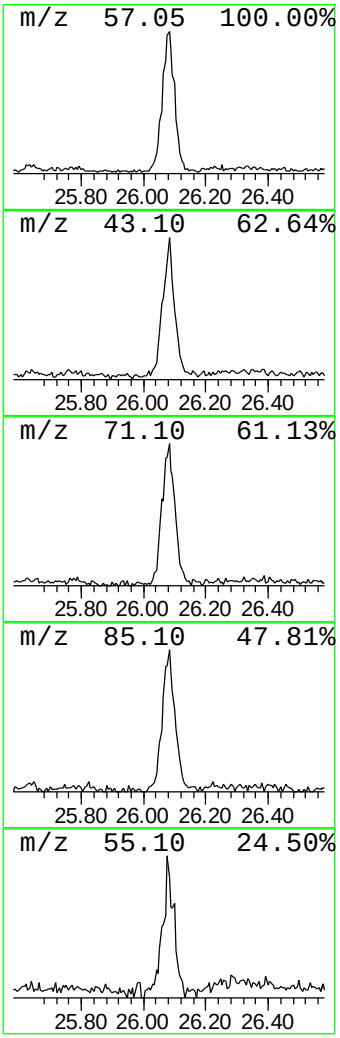
Peak Number 8 Tetratetracontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.08	3.39 ng	283249	Perylene-d12	24.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	87
2	Tetratetracontane	619	C44H90	007098-22-8	87
3	Heneicosane	296	C21H44	000629-94-7	86
4	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	86
5	Tetracosane	338	C24H50	000646-31-1	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG100419\
Data File : BG043032.D
Acq On : 4 Oct 2019 17:39
Operator : JU
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Misc :
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Instrument : BNA_G
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.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
1-Pentene, 2-methyl-	3.17	6.1	ng	127673	1	8.06	420855	20.0
Butane, 2-methoxy...	3.26	6.0	ng	125890	1	8.06	420855	20.0
unknown7.60	7.60	94.4	ng	1985590	1	8.06	420855	20.0
1-Octadecene	21.35	2.3	ng	147193	5	21.69	1288640	20.0
Octacosane	23.19	3.3	ng	209936	5	21.69	1288640	20.0
2-methyloctacosane	24.00	3.6	ng	299268	6	24.91	1672170	20.0
Tetratetracontane	26.08	3.4	ng	283249	6	24.91	1672170	20.0