LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071619\
Data File : BG041662.D
Acq On : 16 Jul 2019 11:02
Operator : HP/JU
Sample : K3778-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : STOCKPILE-COMP

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-BG071519.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	3.118	3	5	13	rVB	231762	340833	5.24%	0.821%
2	3.194	13	18	34	rVB	1071095	1626110	25.00%	3.916%
3	5.609	421	429	445	rBV	1894733	3054255	46.95%	7.356%
4	7.201	691	700	713	rBV	2042401	3562759	54.77%	8.580%
5	7.583	756	765	777	rBV	1937602	3317411	51.00%	7.989%
6	8.047	836	844	852	rBV	376007	654593	10.06%	1.576%
7	8.376	892	900	912	rVB	1357186	2370557	36.44%	5.709%
8	9.205	1033	1041	1055	rBV	1170758	2105516	32.37%	5.071%
9	10.856	1314	1322	1330	rBV	538452	953170	14.65%	2.296%
10	13.300	1730	1738	1745	rBV	2803250	4450861	68.42%	10.719%
11	14.117	1870	1877	1883	rBV	521177	768930	11.82%	1.852%
12	14.669	1961	1971	1981	rBV2	801797	1318745	20.27%	3.176%
13	16.144	2215	2222	2238	rBV	2363230	3618338	55.62%	8.714%
14	17.401	2429	2436	2447	rVB2	1081770	1670905	25.69%	4.024%
15	18.294	2582	2588	2598	rBV	180646	293817	4.52%	0.708%
16	19.563	2799	2804	2811	rBV2	76786	113147	1.74%	0.272%
17	20.010	2874	2880	2891	rVB	4850595	6505210	100.00%	15.666%
18	21.338	3100	3106	3109	rBV4	91882	192241	2.96%	0.463%
19	21.655	3153	3160	3168	rBV	1114084	1788031	27.49%	4.306%
20	21.884	3194	3199	3204	rBV	56717	81895	1.26%	0.197%
21	22.495	3298	3303	3310	rBV	92980	155470	2.39%	0.374%
22	23.194	3417	3422	3429	rVB	102426	197667	3.04%	0.476%
23	24.011	3554	3561	3569	rBV	98262	233234	3.59%	0.562%
24	24.851	3694	3704	3714	rVB	691101	1845929	28.38%	4.446%
25	24.975	3719	3725	3736	rVB3	73008	182453	2.80%	0.439%
26	26.120	3914	3920	3930	rVB4	42969	121052	1.86%	0.292%

Sum of corrected areas: 41523129

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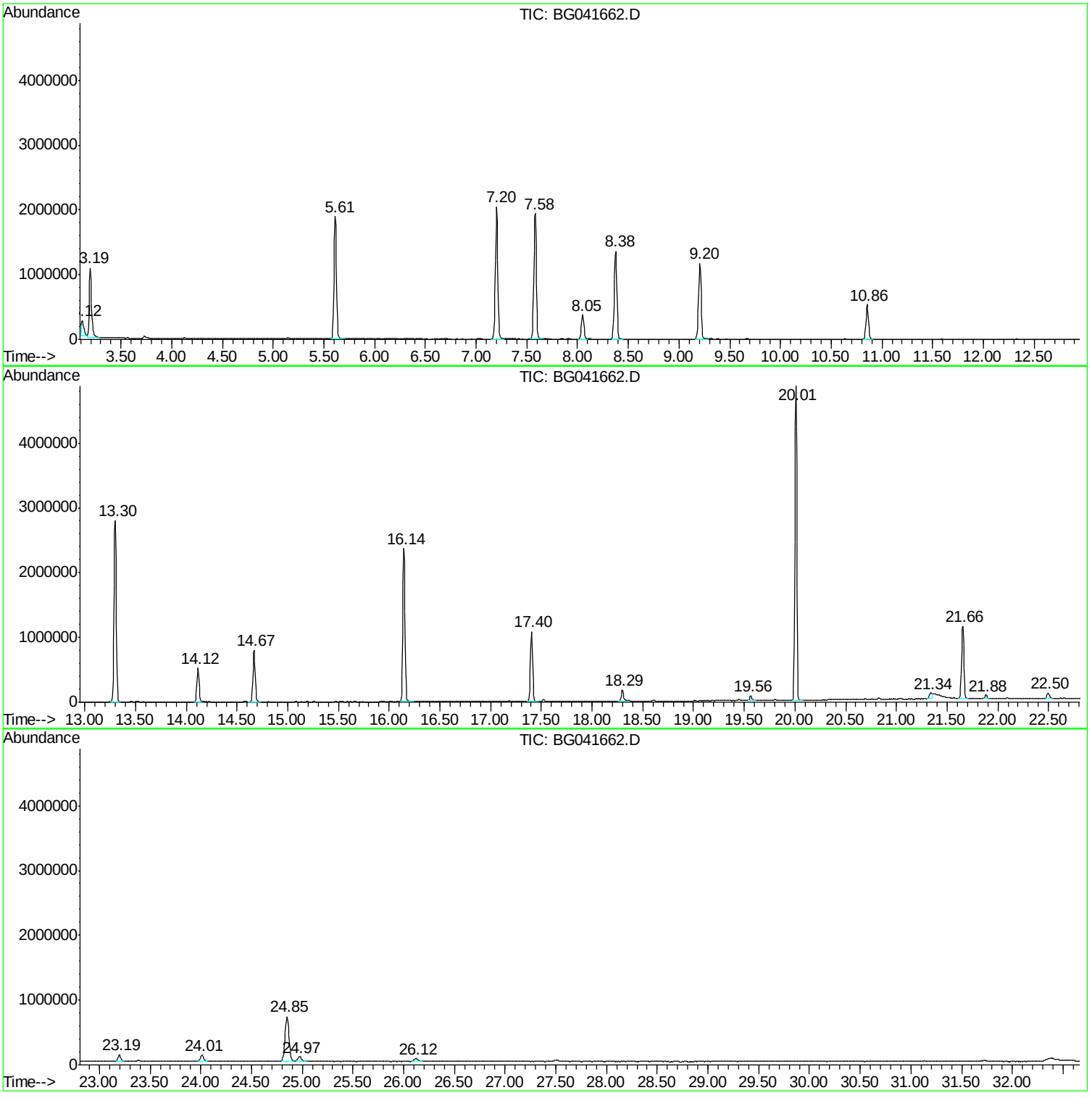
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
STOCKPILE-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.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\BG071619\
Data File : BG041662.D
Acq On : 16 Jul 2019 11:02
Operator : HP/JU
Sample : K3778-01
Misc :
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Instrument : BNA_G
ClientSampleId : STOCKPILE-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

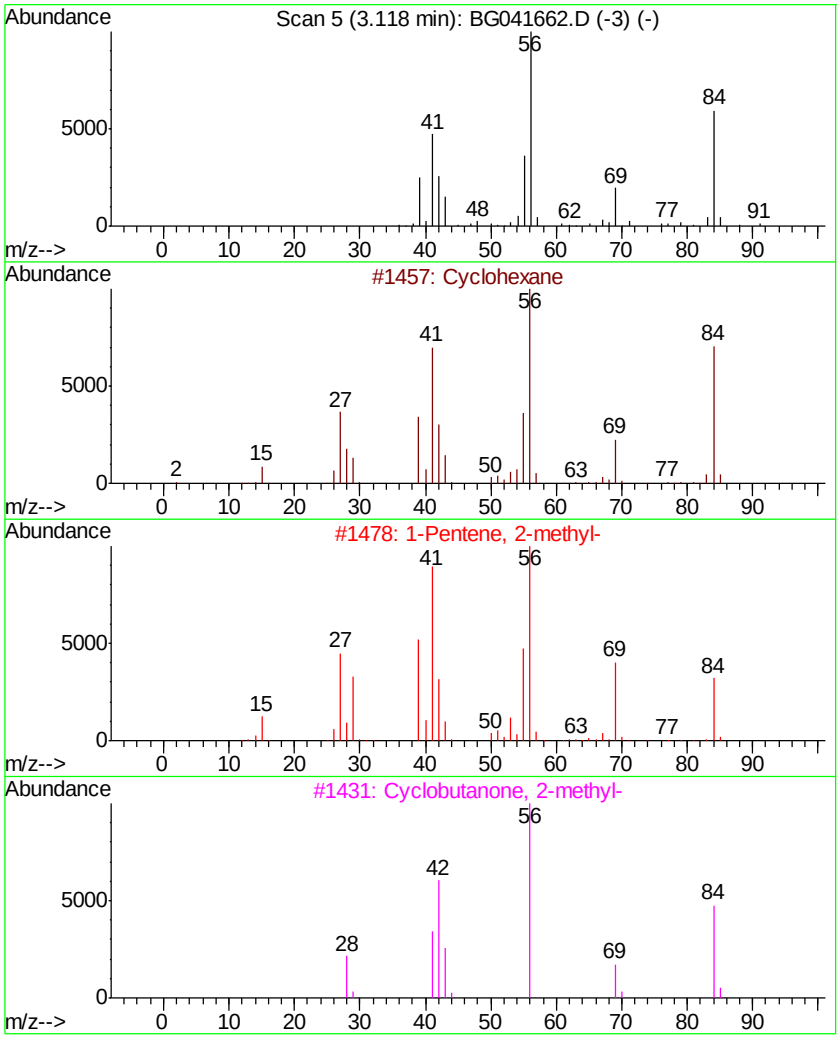
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

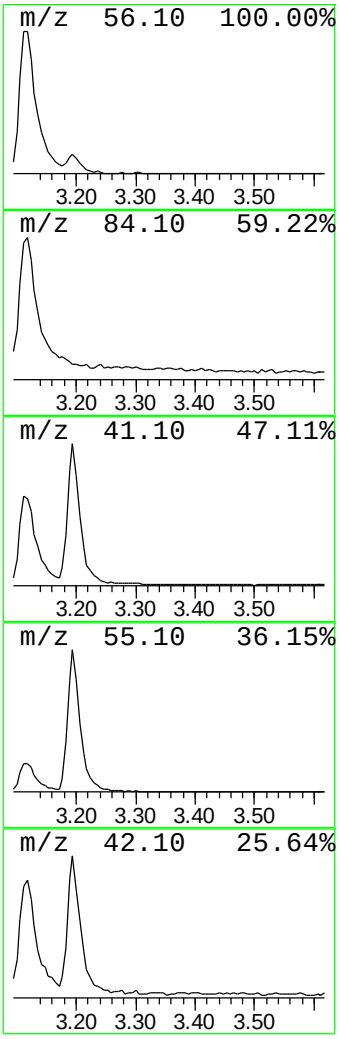
****

Peak Number 1 1-Pentene, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.12	10.41 ng	340833	1,4-Dichlorobenzene-d4	8.05

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	56
3	Cyclobutanone, 2-methyl-	84	C5H8O	001517-15-3	45
4	Cyclopentane, methyl-	84	C6H12	000096-37-7	36
5	2-Acetylpiperidine	127	C7H13NO	097073-22-8	25





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Data File : BG041662.D
Acq On : 16 Jul 2019 11:02
Operator : HP/JU
Sample : K3778-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : STOCKPILE-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

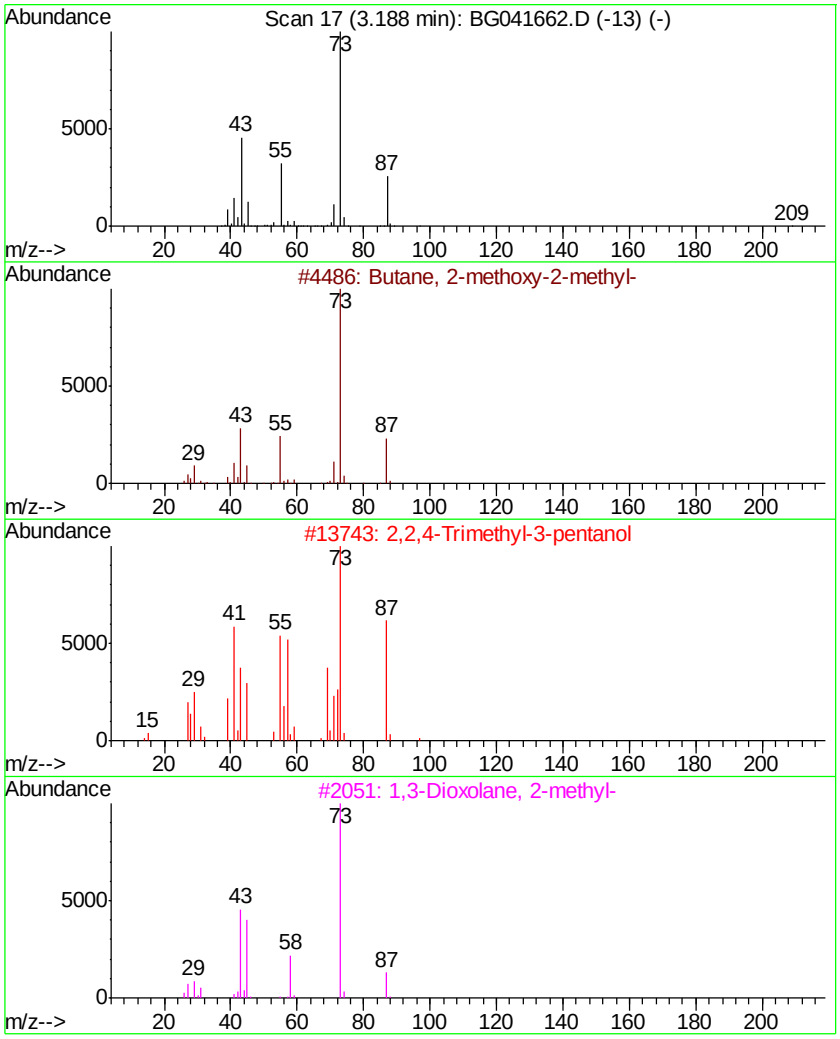
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

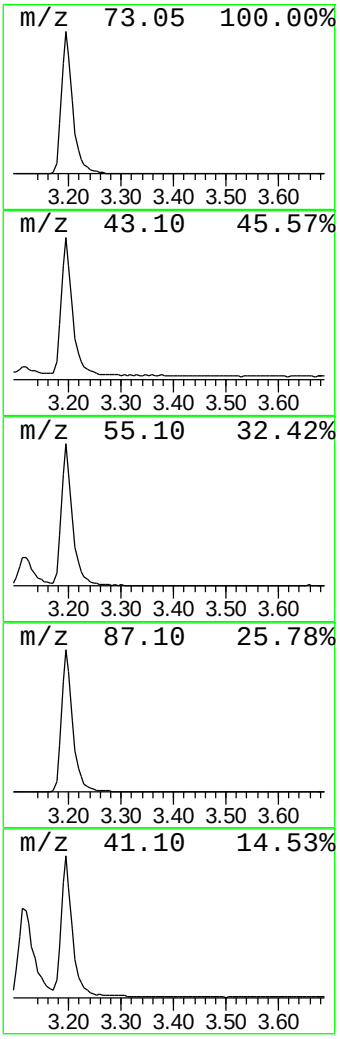
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.19	49.68 ng	1626110	1,4-Dichlorobenzene-d4	8.05

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	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071619\
Data File : BG041662.D
Acq On : 16 Jul 2019 11:02
Operator : HP/JU
Sample : K3778-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : STOCKPILE-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

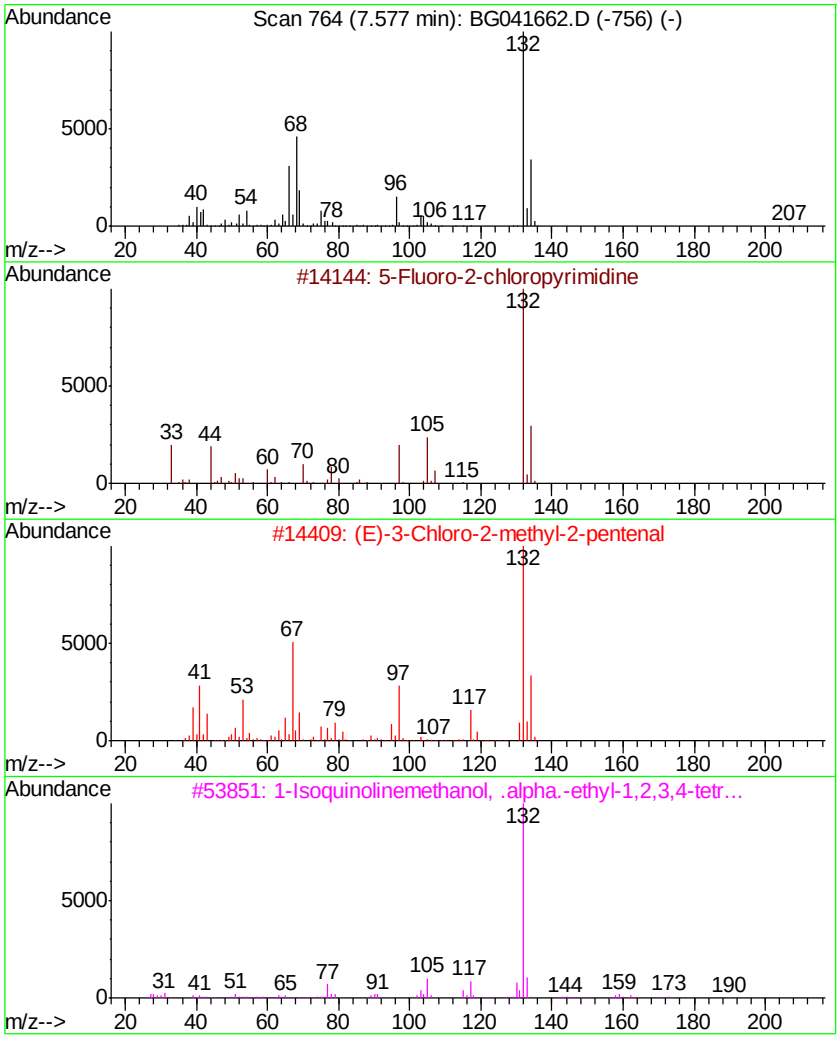
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

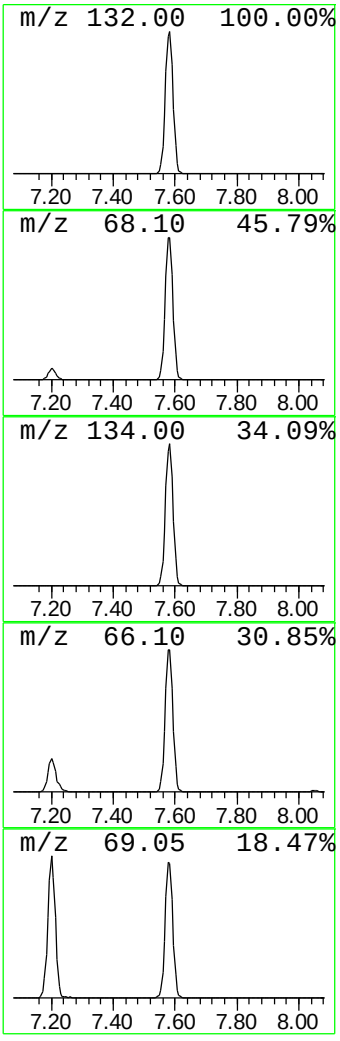
****

Peak Number 3 unknown7.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	101.36 ng	3317410	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	1-Isoquinolinemethanol, .alpha.-...	191	C12H17NO	114608-92-3	12
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	12
5	Amphetaminil	250	C17H18N2	017590-01-1	12





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Acq On : 16 Jul 2019 11:02
Operator : HP/JU
Sample : K3778-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : STOCKPILE-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

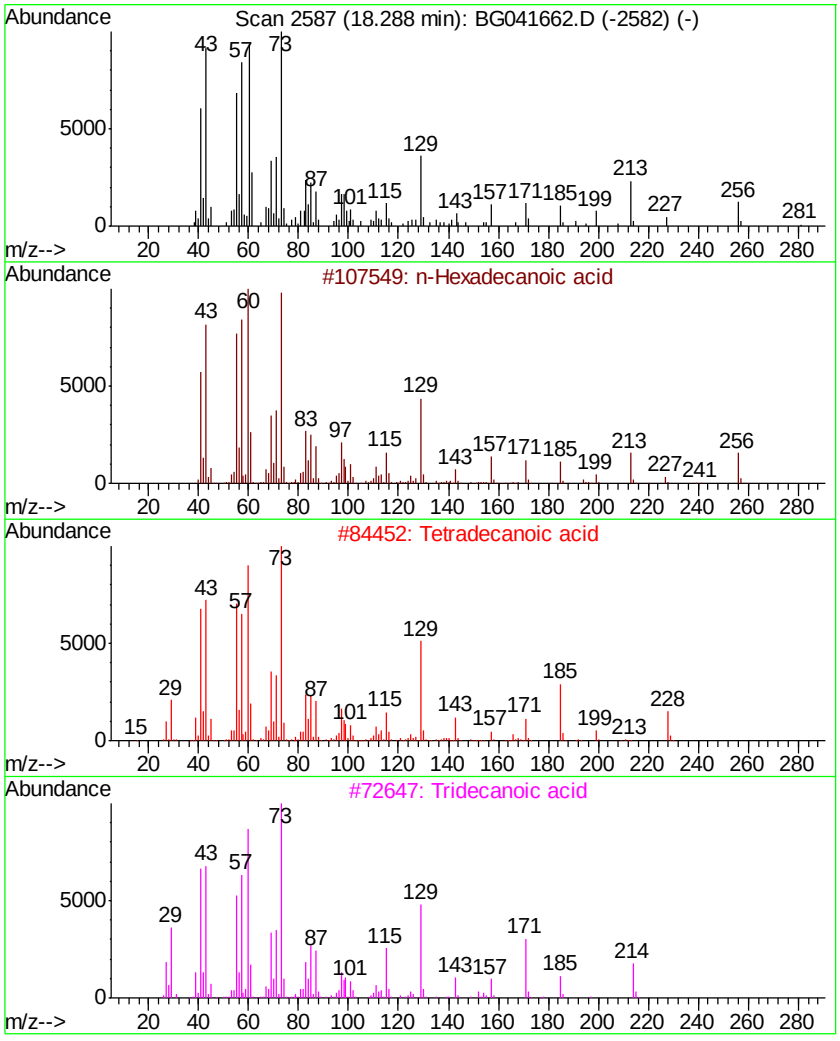
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

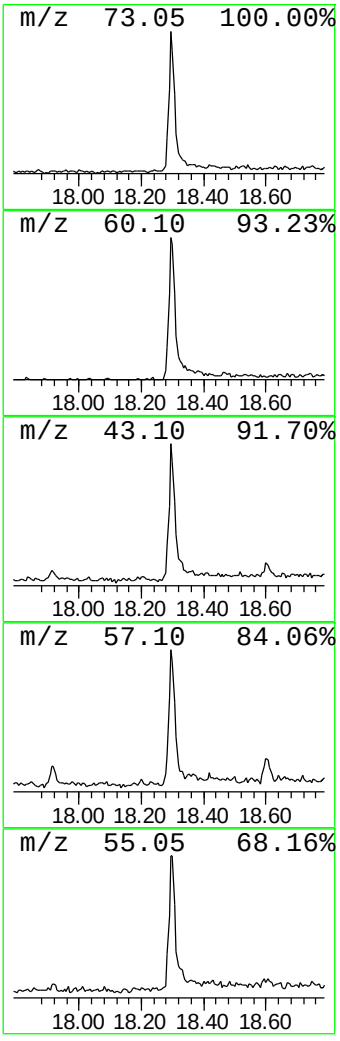
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.29	3.52 ng	293817	Phenanthrene-d10	17.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	95
3	Tridecanoic acid	214	C13H26O2	000638-53-9	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	Undecanoic acid	186	C11H22O2	000112-37-8	59





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Misc :
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Instrument : BNA_G
ClientSampleId : STOCKPILE-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
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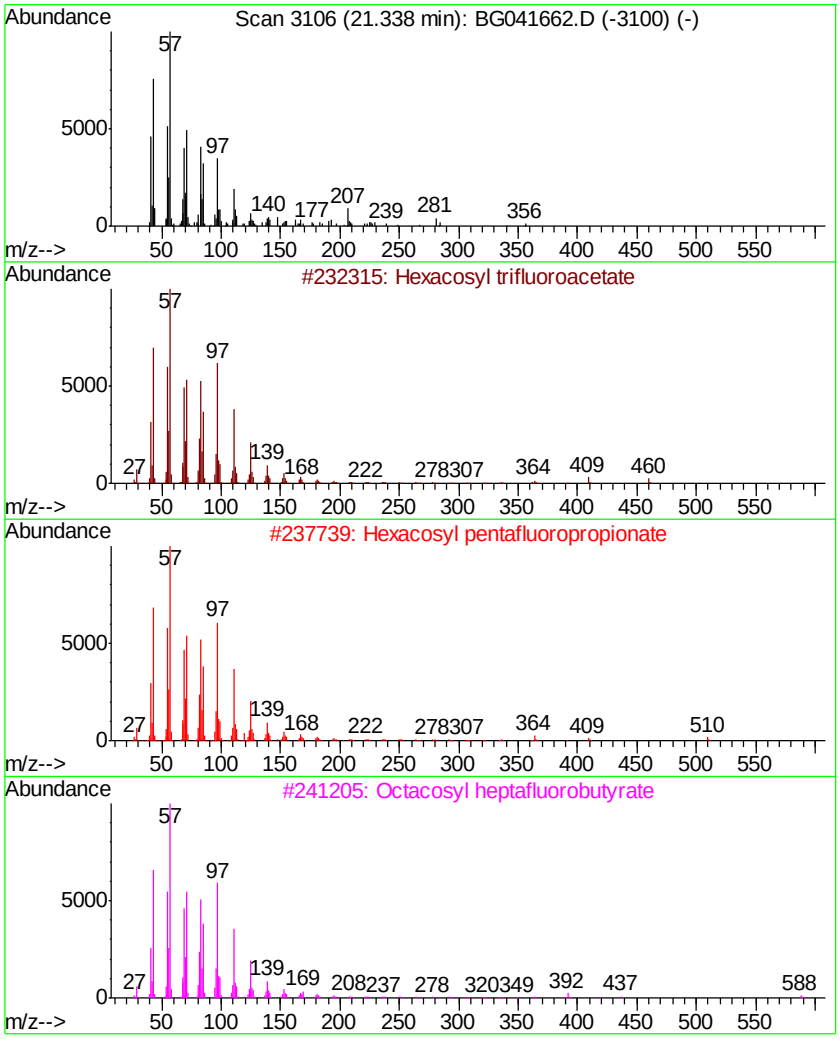
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

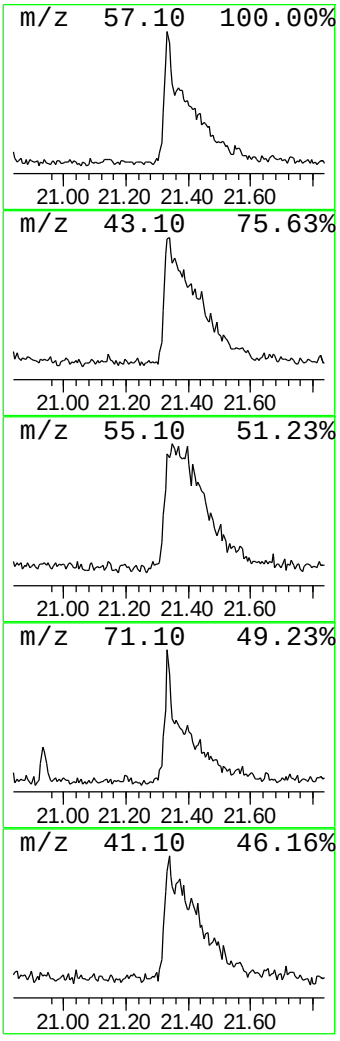
****

Peak Number 6 Hexacosyl trifluoroacetate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.34	2.15 ng	192241	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosyl trifluoroacetate	478	C28H53F3O2	1000351-75-0	87
2	Hexacosyl pentafluoropropionate	528	C29H53F5O2	1000351-81-2	87
3	Octacosyl heptafluorobutyrate	606	C32H57F7O2	1000351-83-6	87
4	Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	87
5	Triacontyl pentafluoropropionate	584	C33H61F5O2	1000351-80-0	87





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Sample : K3778-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : STOCKPILE-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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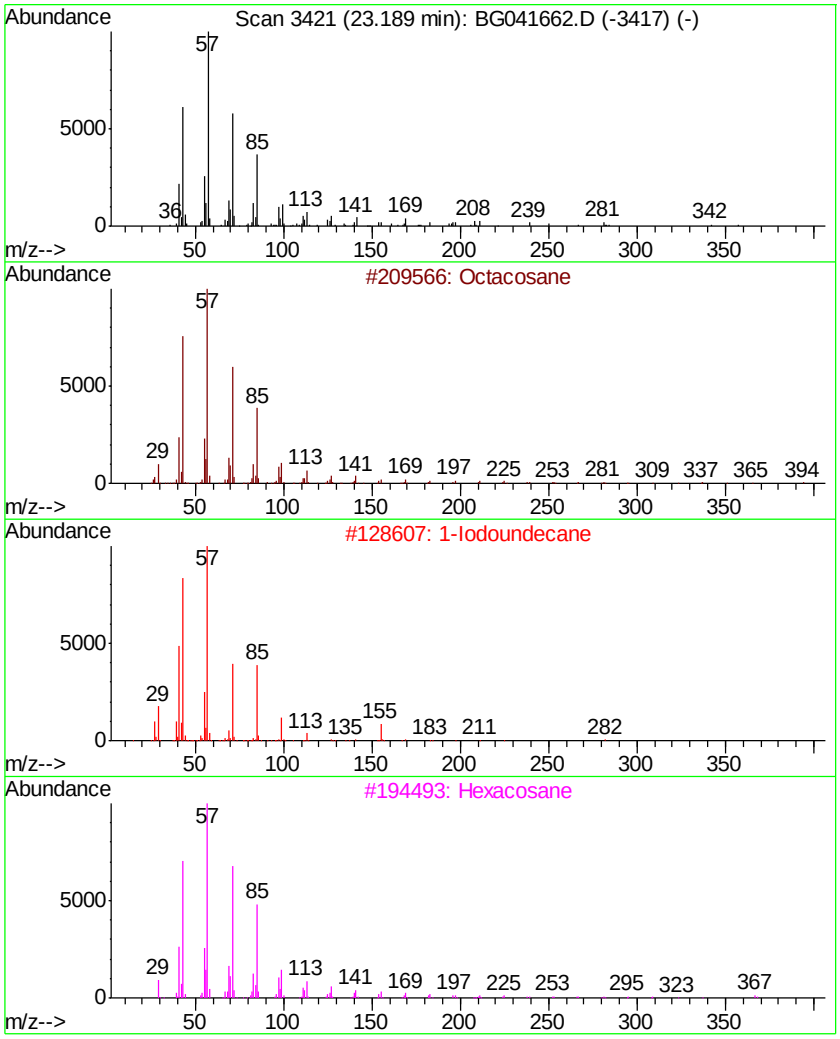
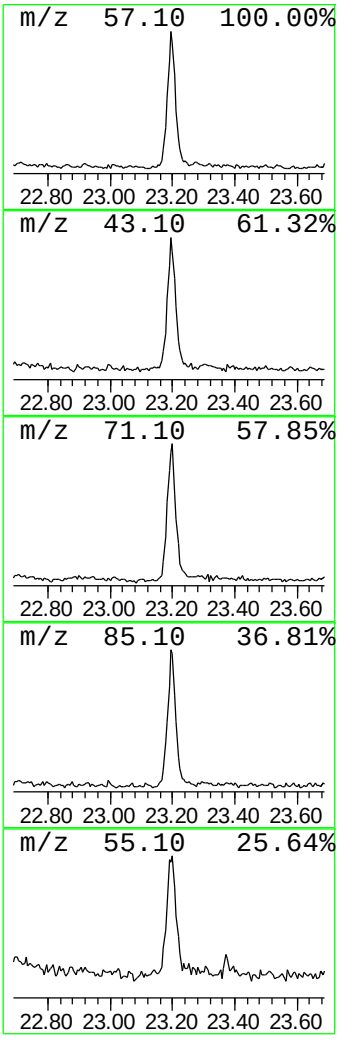
****

Peak Number 7 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.19	2.21 ng	197667	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	90
2	1-Iodoundecane	282	C11H23I	004282-44-4	87
3	Hexacosane	366	C26H54	000630-01-3	87
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	83
5	Nonadecane	268	C19H40	000629-92-5	83





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Sample : K3778-01
Misc :
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Instrument : BNA_G
ClientSampleId : STOCKPILE-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

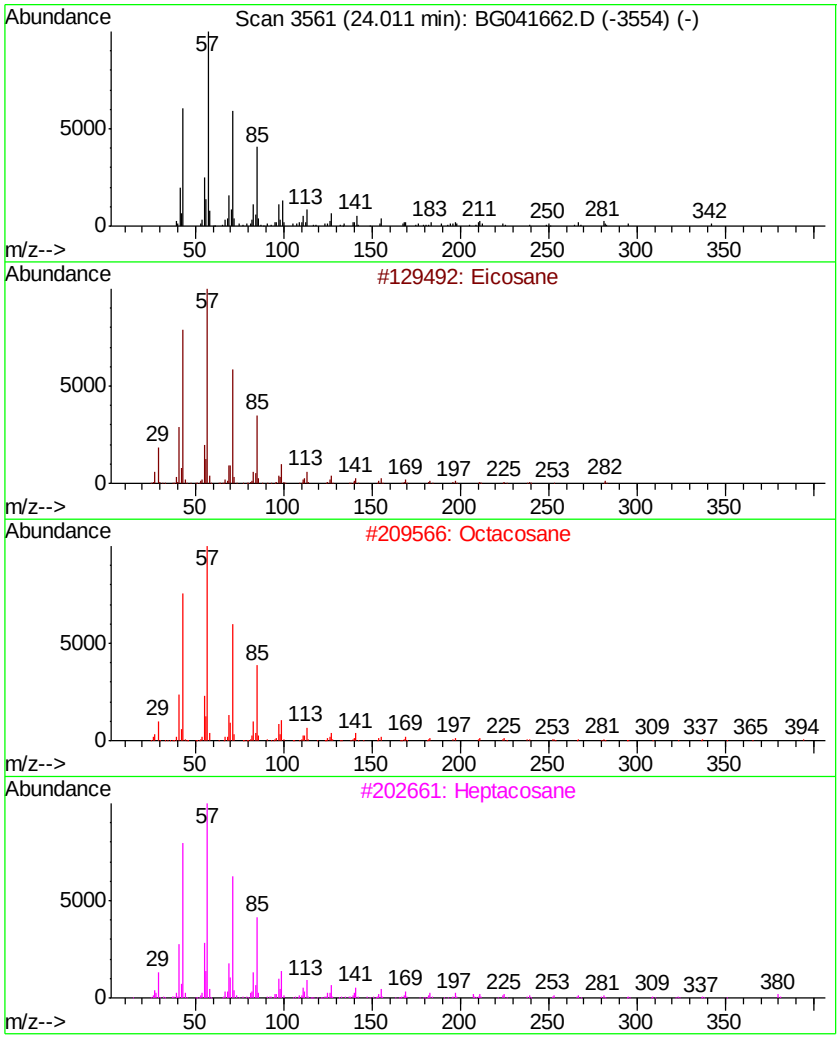
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

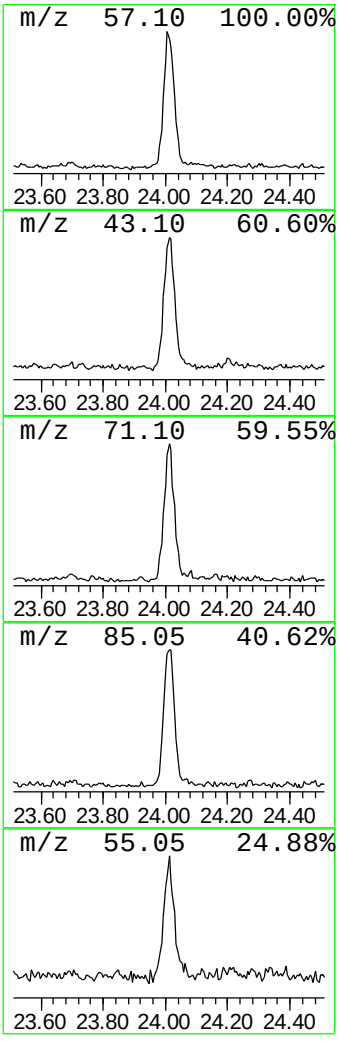
****

Peak Number 8 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.01	2.53 ng	233234	Perylene-d12	24.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Octacosane	394	C28H58	000630-02-4	90
3	Heptacosane	380	C27H56	000593-49-7	90
4	Tetratetracontane	619	C44H90	007098-22-8	90
5	Hentriacontane	437	C31H64	000630-04-6	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG071619\
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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-	3.12	10.4	ng	340833	1	8.05	654593	20.0
Butane, 2-methoxy...	3.19	49.7	ng	1626110	1	8.05	654593	20.0
unknown7.58	7.58	101.4	ng	3317410	1	8.05	654593	20.0
n-Hexadecanoic acid	18.29	3.5	ng	293817	4	17.40	1670910	20.0
Hexacosyl trifluo...	21.34	2.1	ng	192241	5	21.66	1788030	20.0
Octacosane	23.19	2.2	ng	197667	5	21.66	1788030	20.0
Eicosane	24.01	2.5	ng	233234	6	24.85	1845930	20.0