LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG041720\
Data File : BG045056.D
Acq On : 18 Apr 2020 7:46
Operator : CG/JU
Sample : L2283-08
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FB-2020-04-14

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-BG041520.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	3.120	3	5	14	rVB	109594	166803	2.49%	0.625%
2	3.197	14	18	31	rVB	148883	225473	3.37%	0.845%
3	5.594	419	426	436	rBV	427440	718323	10.74%	2.691%
4	7.180	690	696	709	rVB	307766	526403	7.87%	1.972%
5	8.020	830	839	846	rBV	217234	387616	5.79%	1.452%
6	8.349	887	895	905	rBV	909653	1617593	24.18%	6.061%
7	9.183	1025	1037	1045	rBV	803068	1520852	22.73%	5.698%
8	10.828	1309	1317	1327	rVB	322025	588235	8.79%	2.204%
9	13.283	1726	1735	1745	rBV	2535936	4033788	60.30%	15.114%
10	14.106	1869	1875	1880	rBV	148653	223244	3.34%	0.836%
11	14.658	1961	1969	1978	rBV	600363	967510	14.46%	3.625%
12	16.144	2214	2222	2233	rBV	2372000	3670605	54.87%	13.753%
13	17.401	2429	2436	2444	rBV	812816	1263520	18.89%	4.734%
14	20.015	2873	2881	2888	rBV	4780734	6689918	100.00%	25.065%
15	21.319	3097	3103	3112	rBV4	94186	187548	2.80%	0.703%
16	21.660	3155	3161	3171	rVB2	770100	1324189	19.79%	4.961%
17	21.877	3193	3198	3205	rBV2	49340	73931	1.11%	0.277%
18	22.488	3297	3302	3308	rBV3	71609	120962	1.81%	0.453%
19	23.176	3413	3419	3430	rVB2	105214	206811	3.09%	0.775%
20	23.986	3549	3557	3562	rVB2	104250	229616	3.43%	0.860%
21	24.850	3692	3704	3712	rBV2	464275	1354665	20.25%	5.076%
22	24.926	3712	3717	3728	rVB3	99895	254654	3.81%	0.954%
23	26.048	3900	3908	3919	rVB5	71247	212289	3.17%	0.795%
24	27.405	4129	4139	4146	rBV7	38571	125311	1.87%	0.470%

Sum of corrected areas: 26689859

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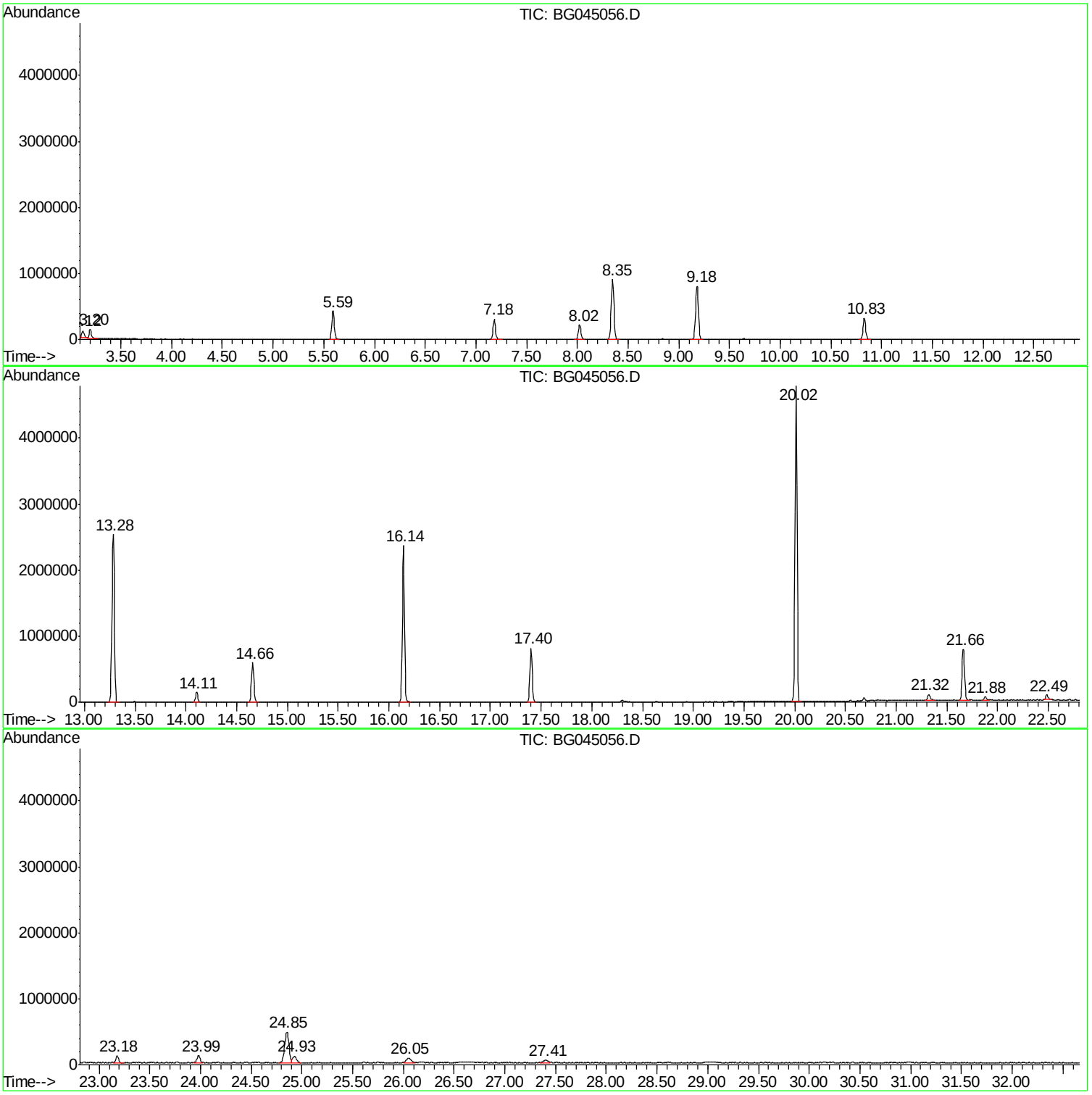
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FB-2020-04-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041520.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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Data File : BG045056.D
Acq On : 18 Apr 2020 7:46
Operator : CG/JU
Sample : L2283-08
Misc :
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Instrument : BNA_G
ClientSampleId : FB-2020-04-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

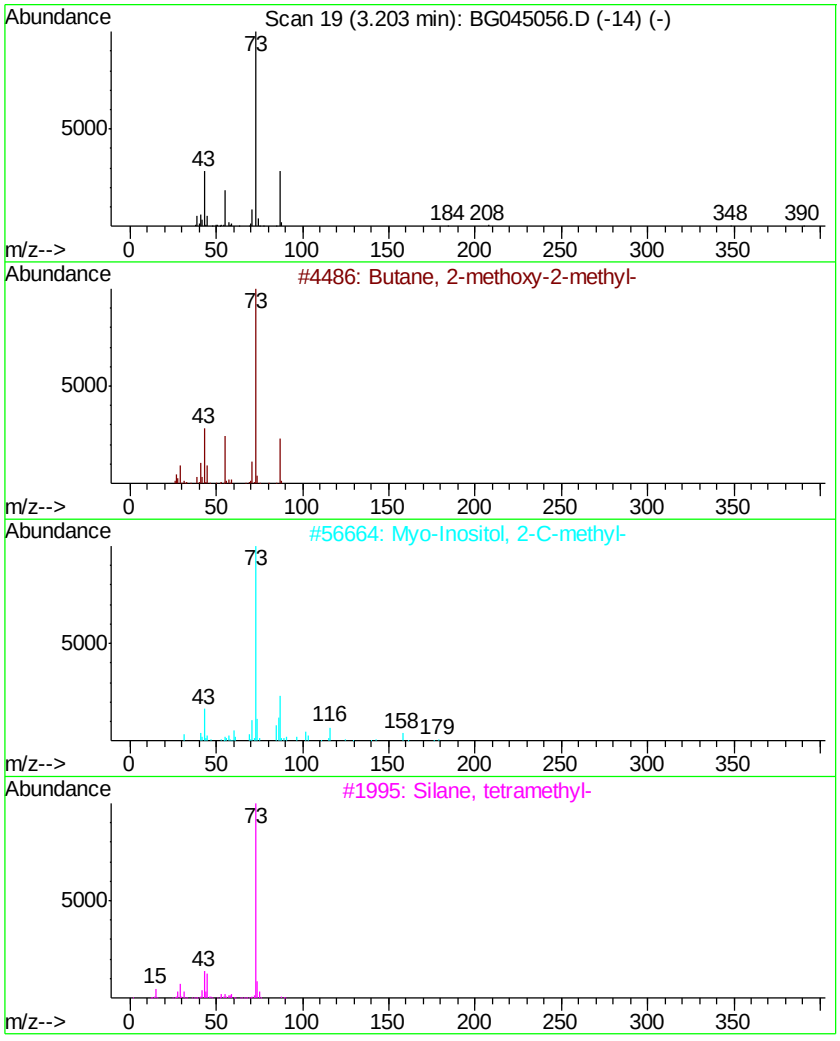
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

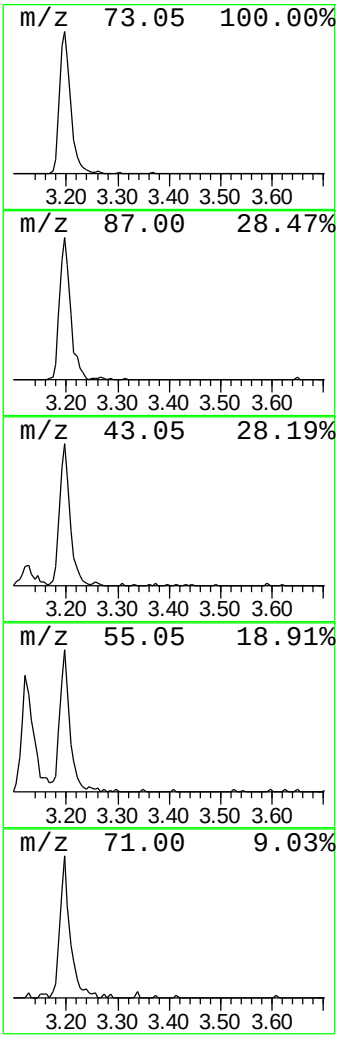
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.20	11.63 ng	225473	1,4-Dichlorobenzene-d4	8.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2	Myo-Inositol, 2-C-methyl-	194	C7H14O6	000472-96-8	38
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	1-Propene-1-thiol	74	C3H6S	000925-89-3	9





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Data File : BG045056.D
Acq On : 18 Apr 2020 7:46
Operator : CG/JU
Sample : L2283-08
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FB-2020-04-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

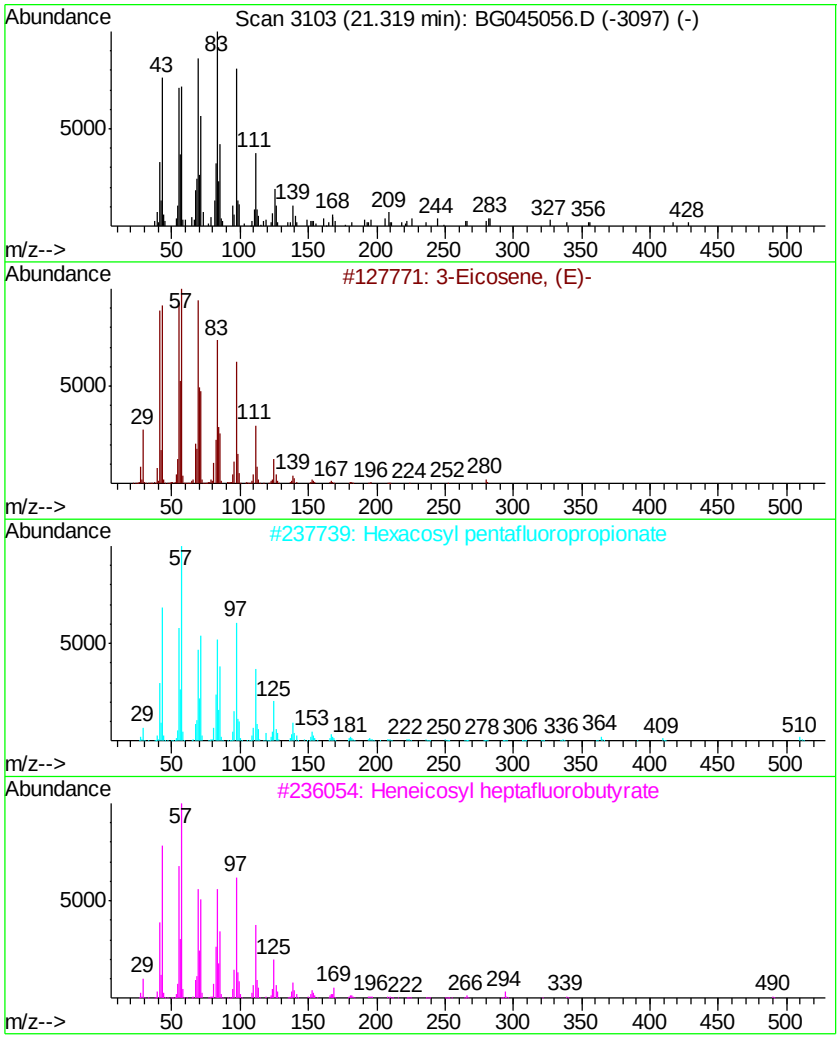
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

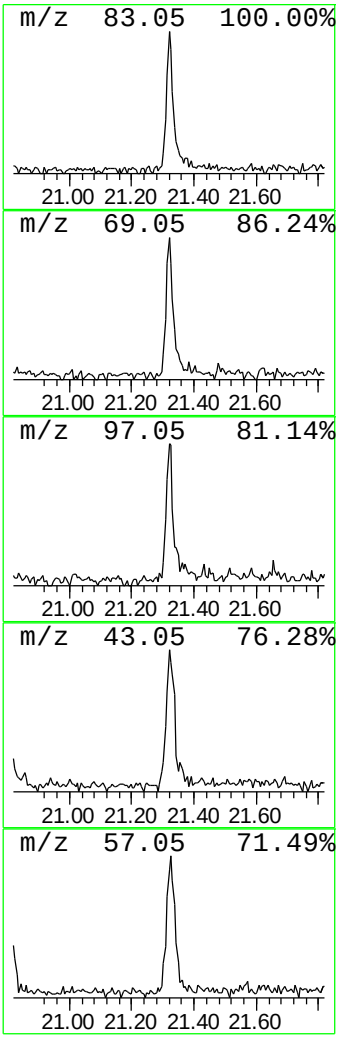
****

Peak Number 4 3-Eicosene, (E)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.32	2.83 ng	187548	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	70
2	Hexacosyl pentafluoropropionate	528	C29H53F5O2	1000351-81-2	64
3	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	64
4	Heptacosyl pentafluoropropionate	542	C30H55F5O2	1000351-81-6	64
5	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	64





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG041720\
Data File : BG045056.D
Acq On : 18 Apr 2020 7:46
Operator : CG/JU
Sample : L2283-08
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FB-2020-04-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

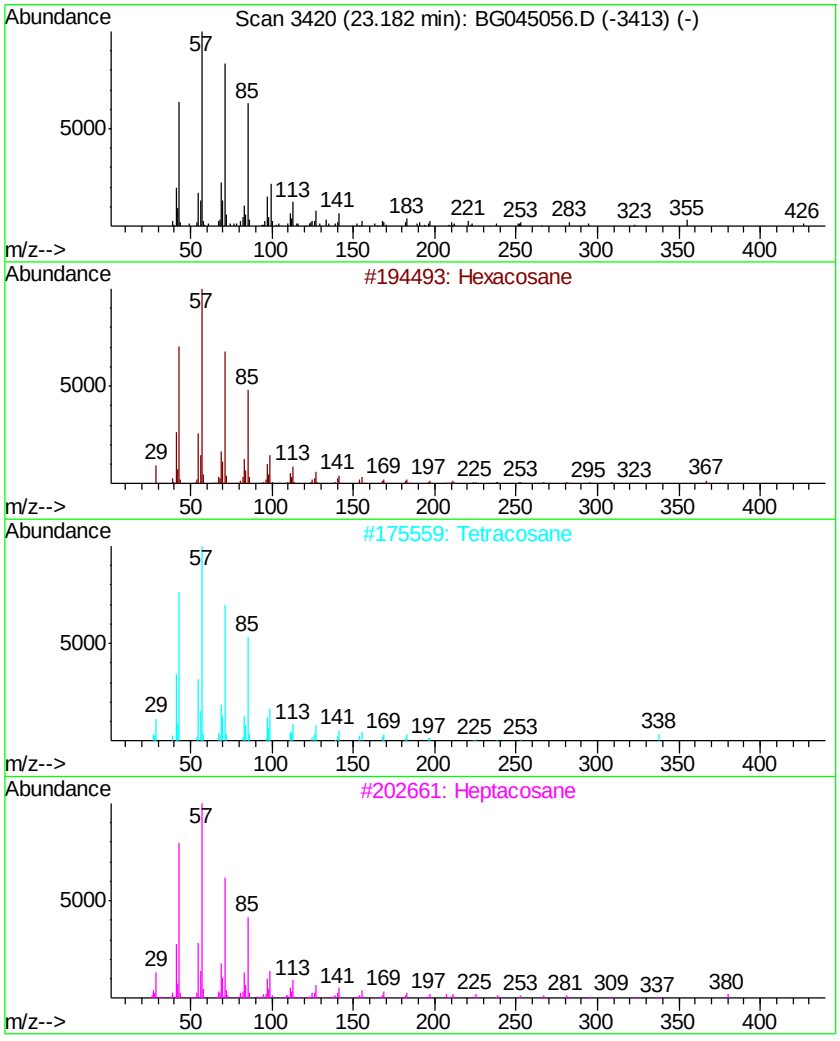
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

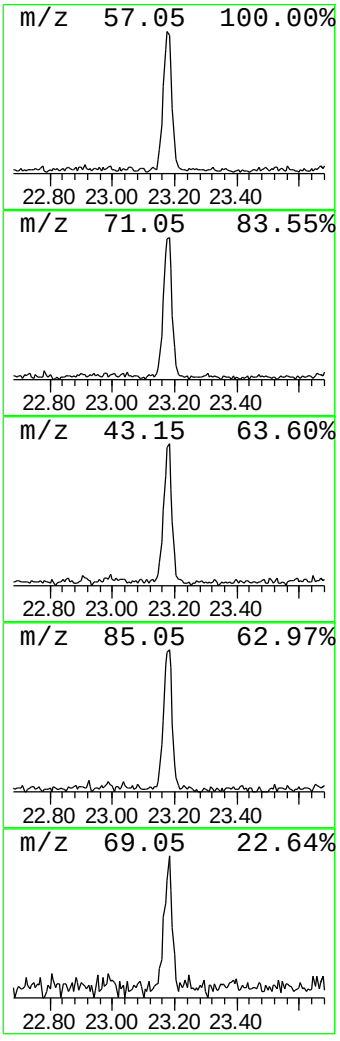
****

Peak Number 5 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.18	3.12 ng	206811	Chrysene-d12	21.66

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	Heptacosane	380	C27H56	000593-49-7	91
4	Heptadecane	240	C17H36	000629-78-7	90
5	Octadecane	254	C18H38	000593-45-3	86





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG041720\
Data File : BG045056.D
Acq On : 18 Apr 2020 7:46
Operator : CG/JU
Sample : L2283-08
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FB-2020-04-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041520.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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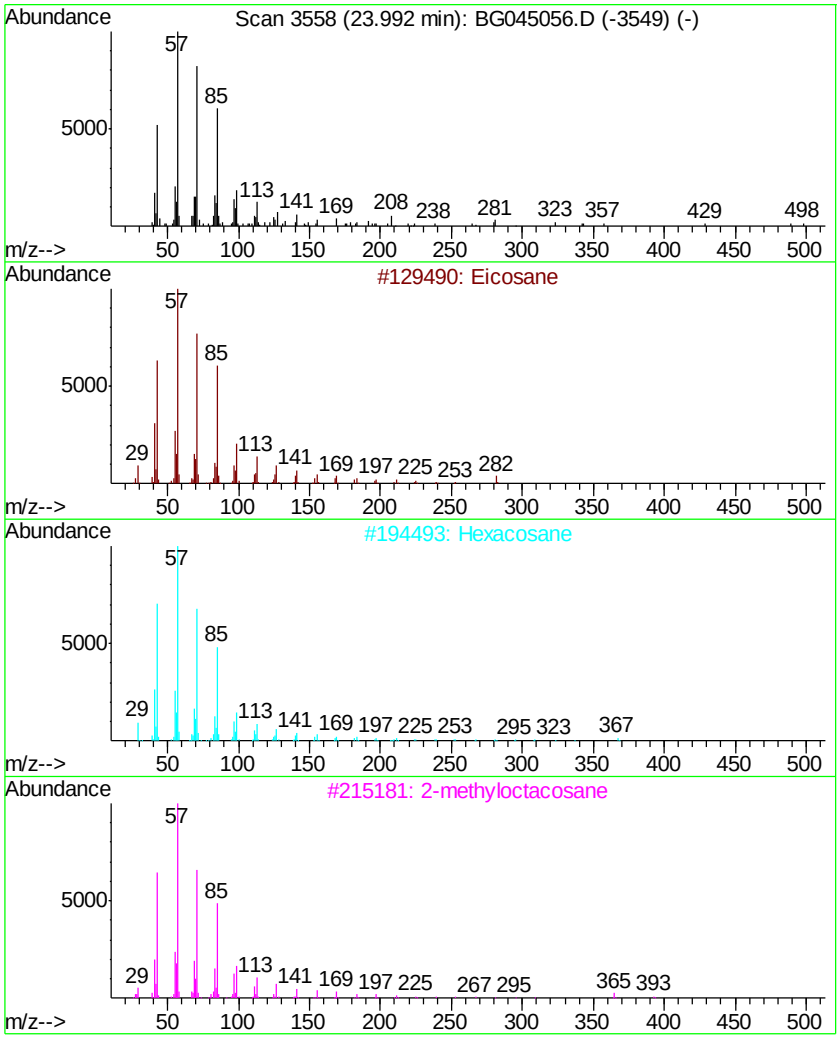
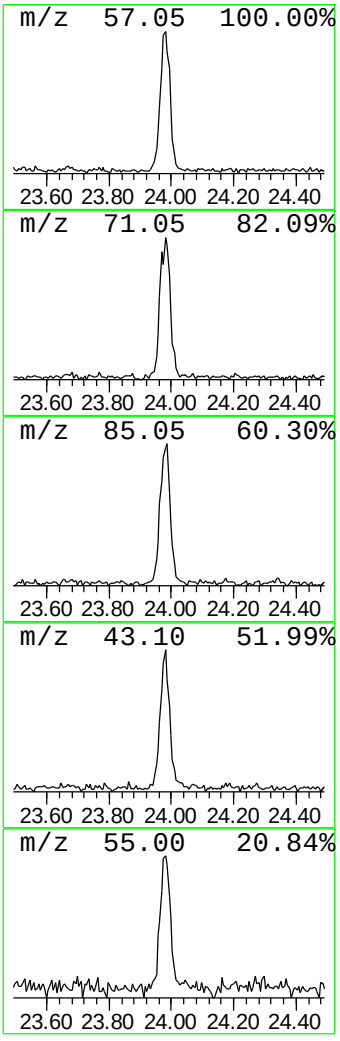
Peak Number 6 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.99	3.39 ng	229616	Perylene-d12	24.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	96
2	Hexacosane	366	C26H54	000630-01-3	90
3	2-methyloctacosane	408	C29H60	1000376-72-8	86
4	Heptacosane	380	C27H56	000593-49-7	86
5	Tetracosane	338	C24H50	000646-31-1	86





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG041720\
Data File : BG045056.D
Acq On : 18 Apr 2020 7:46
Operator : CG/JU
Sample : L2283-08
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FB-2020-04-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

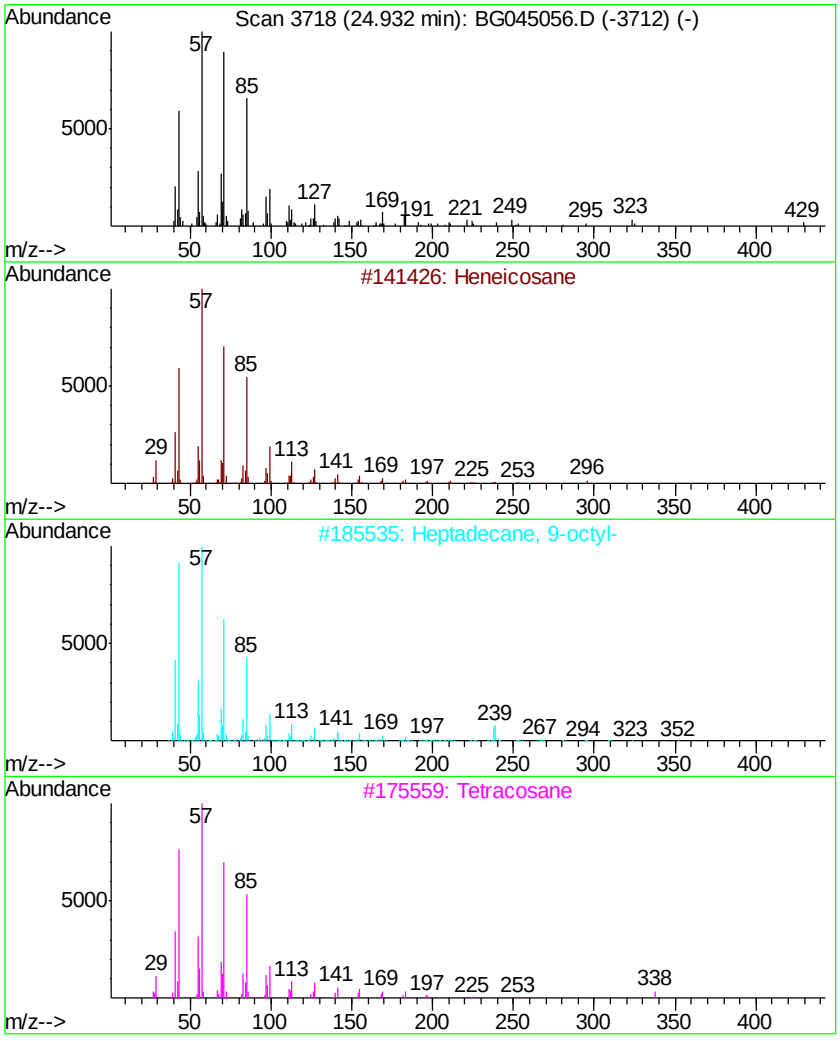
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

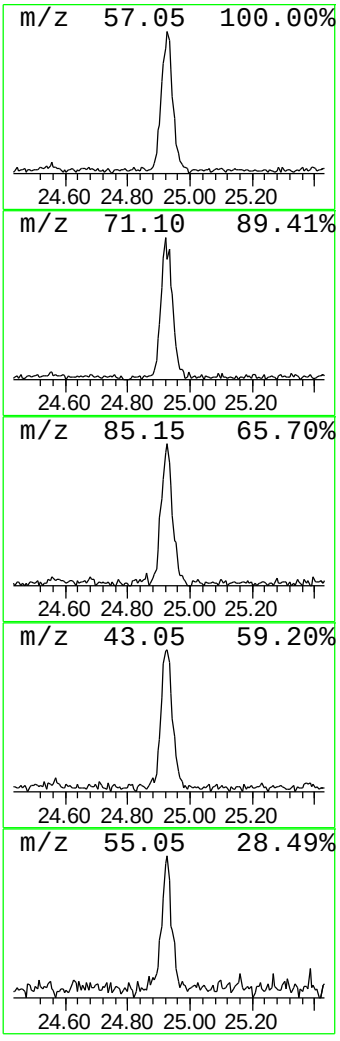
****

Peak Number 7 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.93	3.76 ng	254654	Perylene-d12	24.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
3	Tetracosane	338	C24H50	000646-31-1	80
4	Eicosane	282	C20H42	000112-95-8	80
5	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	72





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG041720\
Data File : BG045056.D
Acq On : 18 Apr 2020 7:46
Operator : CG/JU
Sample : L2283-08
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FB-2020-04-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

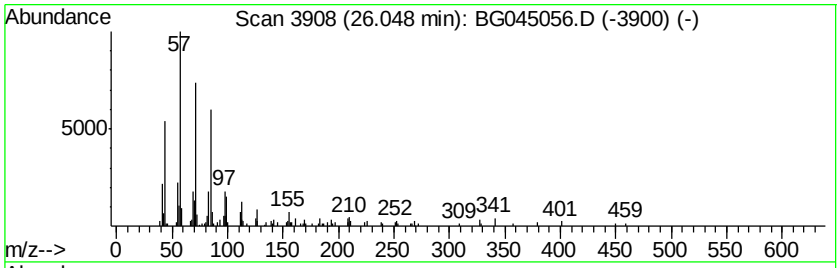
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

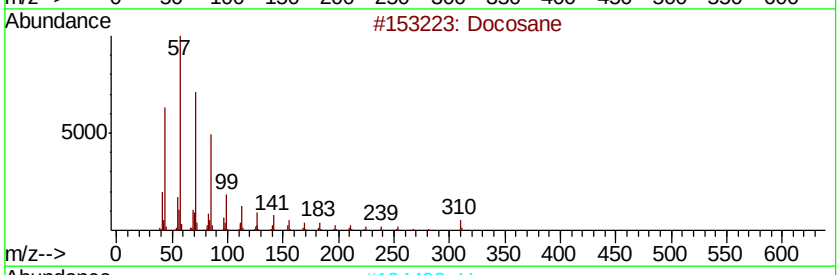
****

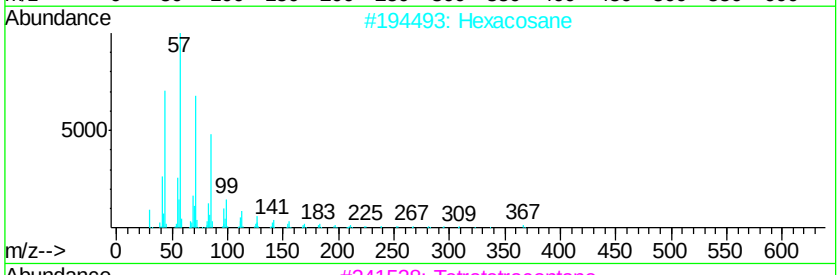
Peak Number 8 Docosane Concentration Rank 6

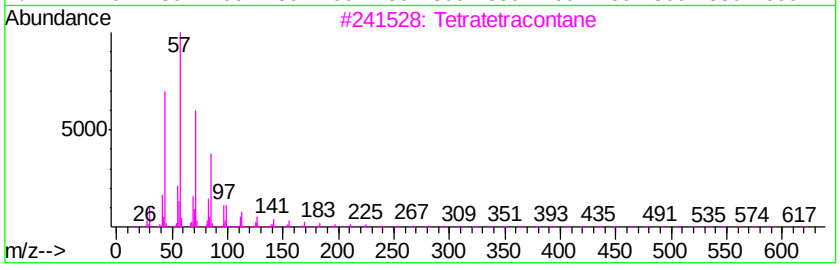
R.T.	EstConc	Area	Relative to ISTD	R.T.
26.05	3.13 ng	212289	Perylene-d12	24.85

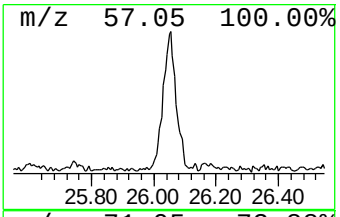
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	74
2	Hexacosane	366	C26H54	000630-01-3	74
3	Tetratetracontane	619	C44H90	007098-22-8	74
4	Triacontane	422	C30H62	000638-68-6	74
5	Hexadecane	226	C16H34	000544-76-3	72

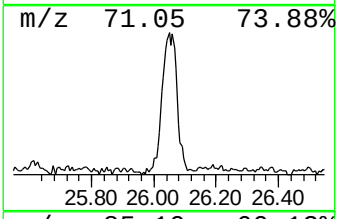


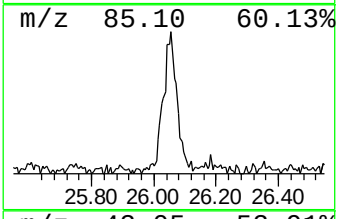


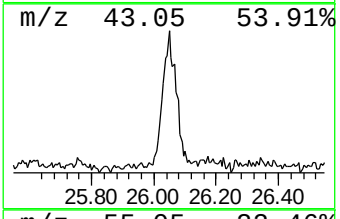


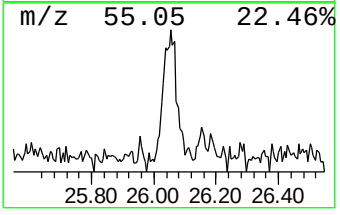












Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG041720\
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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
Butane, 2-methoxy...	3.20	11.6	ng	225473	1	8.02	387616	20.0
3-Eicosene, (E)-	21.32	2.8	ng	187548	5	21.66	1324190	20.0
Hexacosane	23.18	3.1	ng	206811	5	21.66	1324190	20.0
Eicosane	23.99	3.4	ng	229616	6	24.85	1354670	20.0
Heneicosane	24.93	3.8	ng	254654	6	24.85	1354670	20.0
Docosane	26.05	3.1	ng	212289	6	24.85	1354670	20.0