LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG040119\
Data File : BG040290.D
Acq On : 2 Apr 2019 8:26
Operator : JU/SJ
Sample : K2180-31
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-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:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG032719.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	3.122	3	6	14	rVB	83602	139088	3.69%	0.579%
2	5.608	422	429	441	rBV	968853	1554055	41.24%	6.465%
3	7.206	693	701	716	rBV	1025728	1791621	47.54%	7.453%
4	7.582	757	765	778	rBV	967367	1659794	44.04%	6.905%
5	8.052	838	845	855	rBV	198861	328894	8.73%	1.368%
6	8.375	891	900	908	rBV	683327	1173231	31.13%	4.881%
7	9.227	1035	1045	1056	rBV	570181	1041592	27.64%	4.333%
8	10.866	1315	1324	1333	rBV	269033	489578	12.99%	2.037%
9	13.305	1729	1739	1750	rBV	1625420	2530950	67.16%	10.529%
10	14.127	1873	1879	1885	rBV	98254	141213	3.75%	0.587%
11	14.685	1967	1974	1982	rBV2	479059	789178	20.94%	3.283%
12	16.172	2220	2227	2240	rBV	1432479	2194801	58.24%	9.131%
13	17.429	2434	2441	2452	rVB2	679321	1042923	27.68%	4.339%
14	18.293	2579	2588	2596	rBV4	41972	83854	2.23%	0.349%
15	20.032	2878	2884	2891	rBV	2873969	3768446	100.00%	15.677%
16	20.796	3009	3014	3020	rBV3	27027	39773	1.06%	0.165%
17	21.307	3096	3101	3112	rBV4	106276	264326	7.01%	1.100%
18	21.707	3162	3169	3177	rBV	687346	1144656	30.37%	4.762%
19	21.853	3189	3194	3199	rVB	118333	168843	4.48%	0.702%
20	22.470	3293	3299	3306	rBV	189187	304994	8.09%	1.269%
21	23.175	3412	3419	3426	rBV2	234222	461594	12.25%	1.920%
22	23.998	3550	3559	3568	rBV	236191	559296	14.84%	2.327%
23	25.009	3714	3731	3749	rVB3	377975	1672597	44.38%	6.958%
24	26.142	3914	3924	3937	rVB3	122495	427769	11.35%	1.780%
25	27.541	4150	4162	4177	rVB3	62335	264701	7.02%	1.101%

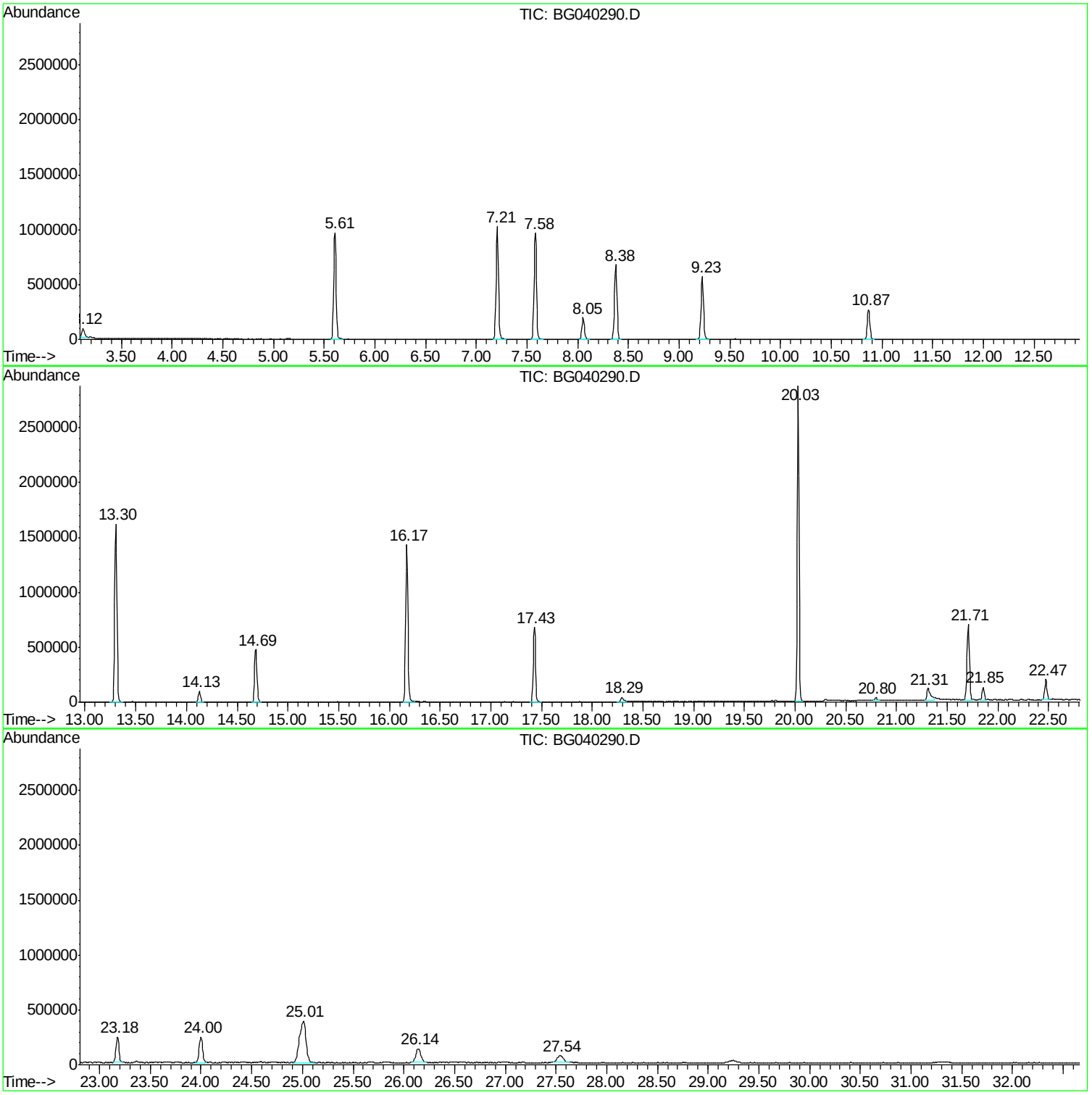
Sum of corrected areas: 24037767

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG040119\
Data File : BG040290.D
Acq On : 2 Apr 2019 8:26
Operator : JU/SJ
Sample : K2180-31
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG032719.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\BG040119\
Data File : BG040290.D
Acq On : 2 Apr 2019 8:26
Operator : JU/SJ
Sample : K2180-31
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG032719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

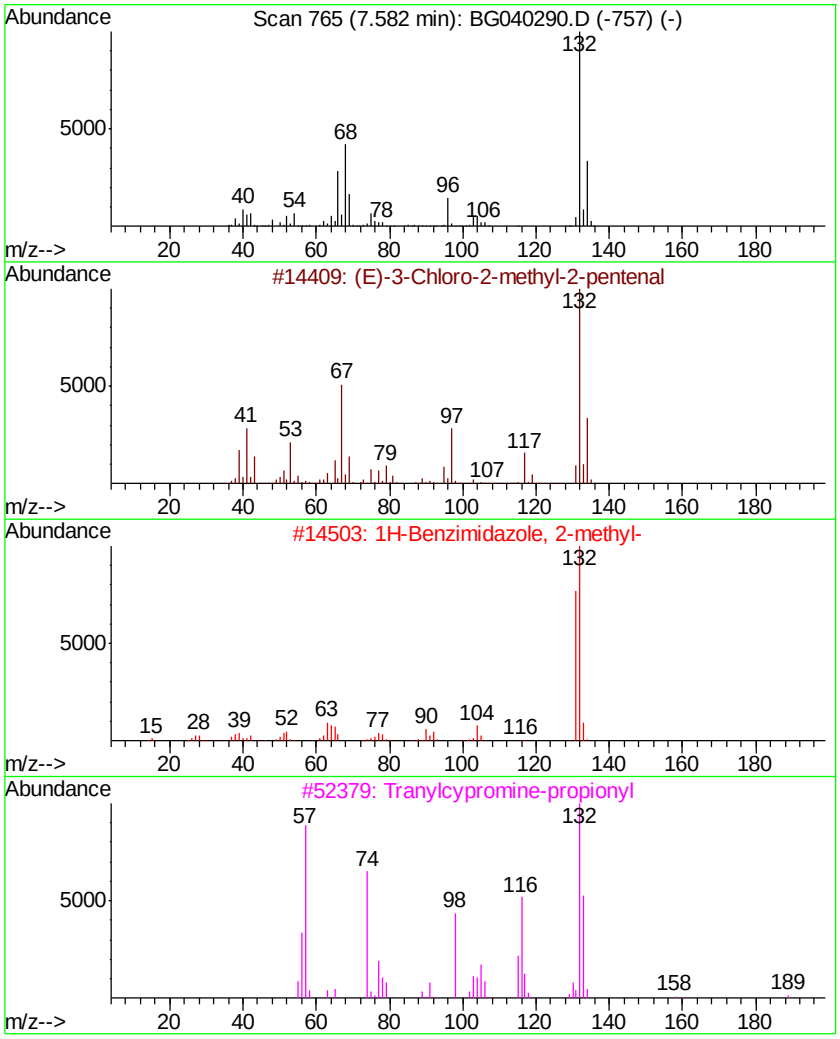
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

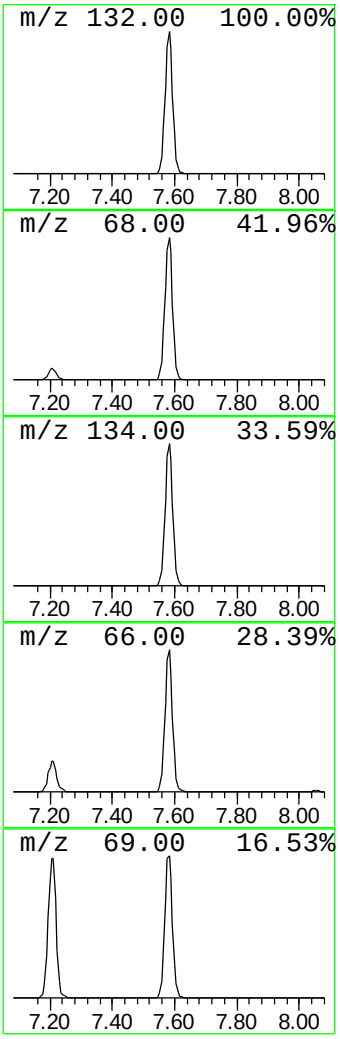
****

Peak Number 2 unknown7.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	100.93 ng	1659790	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG040119\
Data File : BG040290.D
Acq On : 2 Apr 2019 8:26
Operator : JU/SJ
Sample : K2180-31
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG032719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

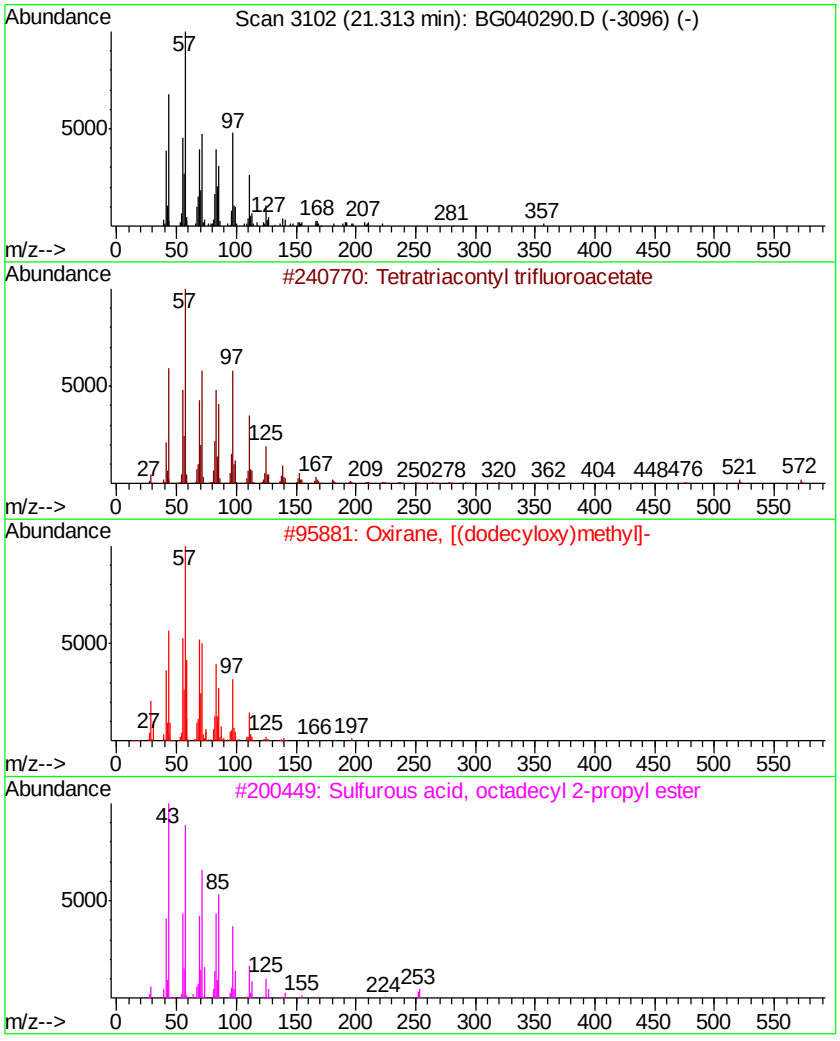
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

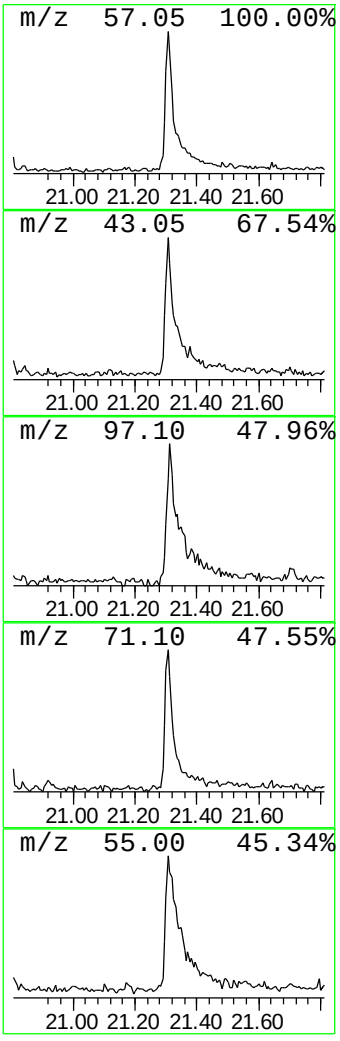
****

Peak Number 4 Tetratriacontyl trifluoroac... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.31	4.62 ng	264326	Chrysene-d12	21.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratriacontyl trifluoroacetate	591	C36H69F3O2	1000351-75-3	90
2	Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	86
3	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	74
4	Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	72
5	Carbonic acid, isobutyl pentadec...	328	C20H40O3	1000314-61-2	72





Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG040119\
Data File : BG040290.D
Acq On : 2 Apr 2019 8:26
Operator : JU/SJ
Sample : K2180-31
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG032719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

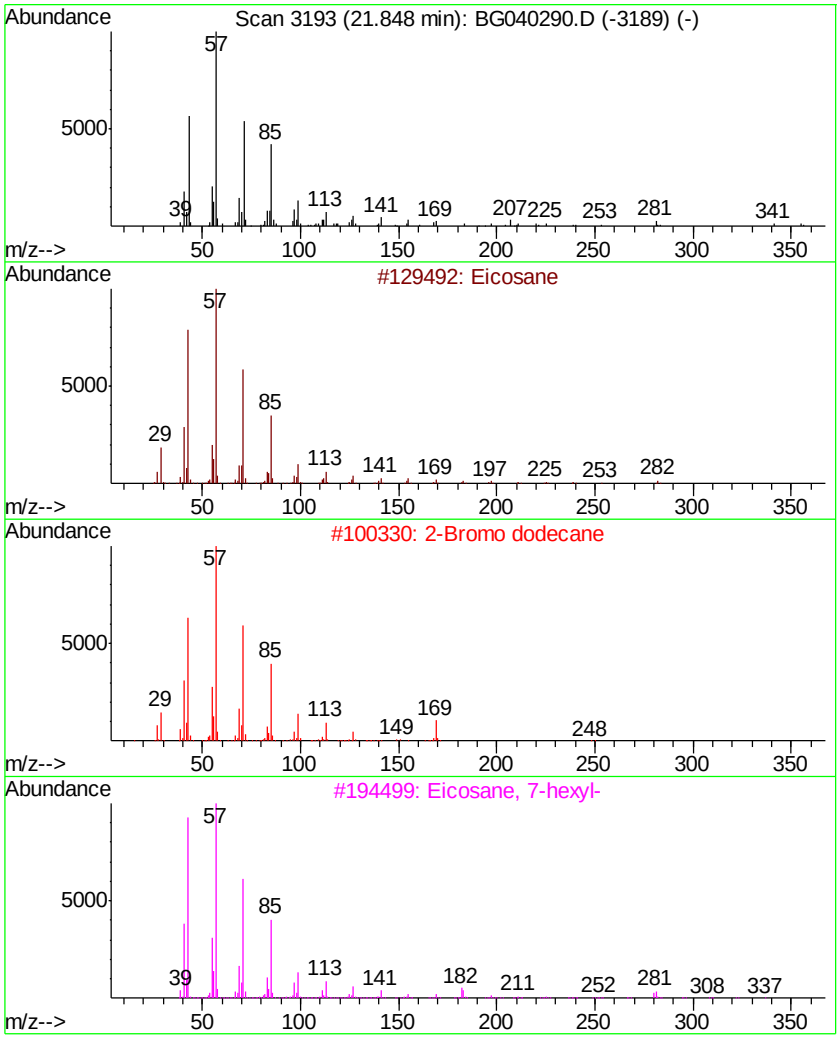
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

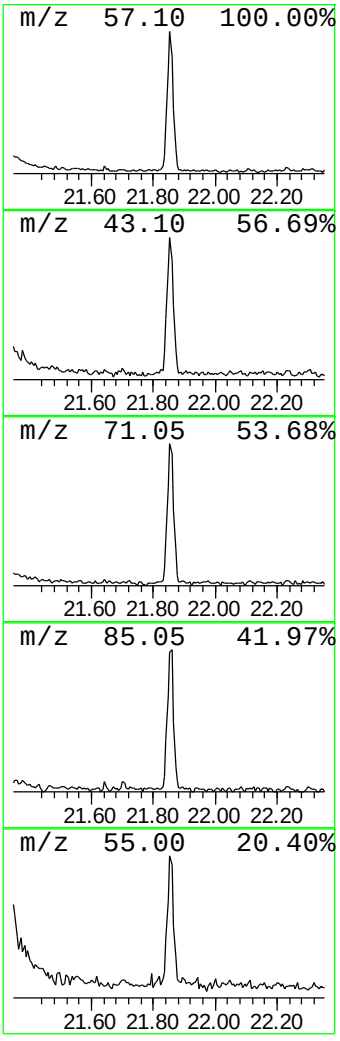
****

Peak Number 5 2-Bromo dodecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.85	2.95 ng	168843	Chrysene-d12	21.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	2-Bromo dodecane	248	C12H25Br	013187-99-0	91
3	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Hexadecane	226	C16H34	000544-76-3	86





Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG040119\
Data File : BG040290.D
Acq On : 2 Apr 2019 8:26
Operator : JU/SJ
Sample : K2180-31
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG032719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

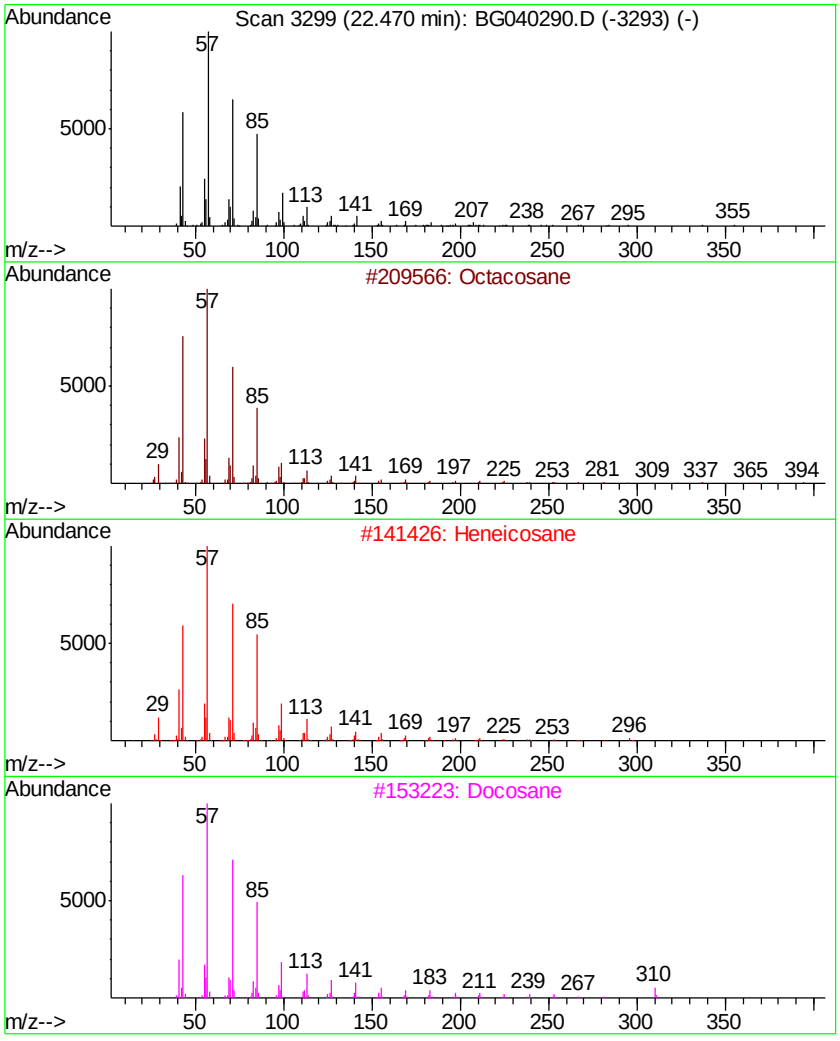
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

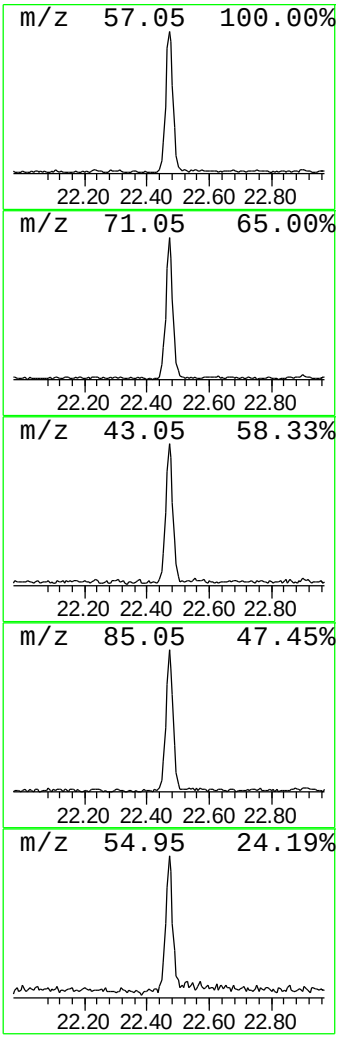
****

Peak Number 6 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.47	5.33 ng	304994	Chrysene-d12	21.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Docosane	310	C22H46	000629-97-0	91
4	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87
5	Eicosane	282	C20H42	000112-95-8	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG040119\
Data File : BG040290.D
Acq On : 2 Apr 2019 8:26
Operator : JU/SJ
Sample : K2180-31
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG032719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

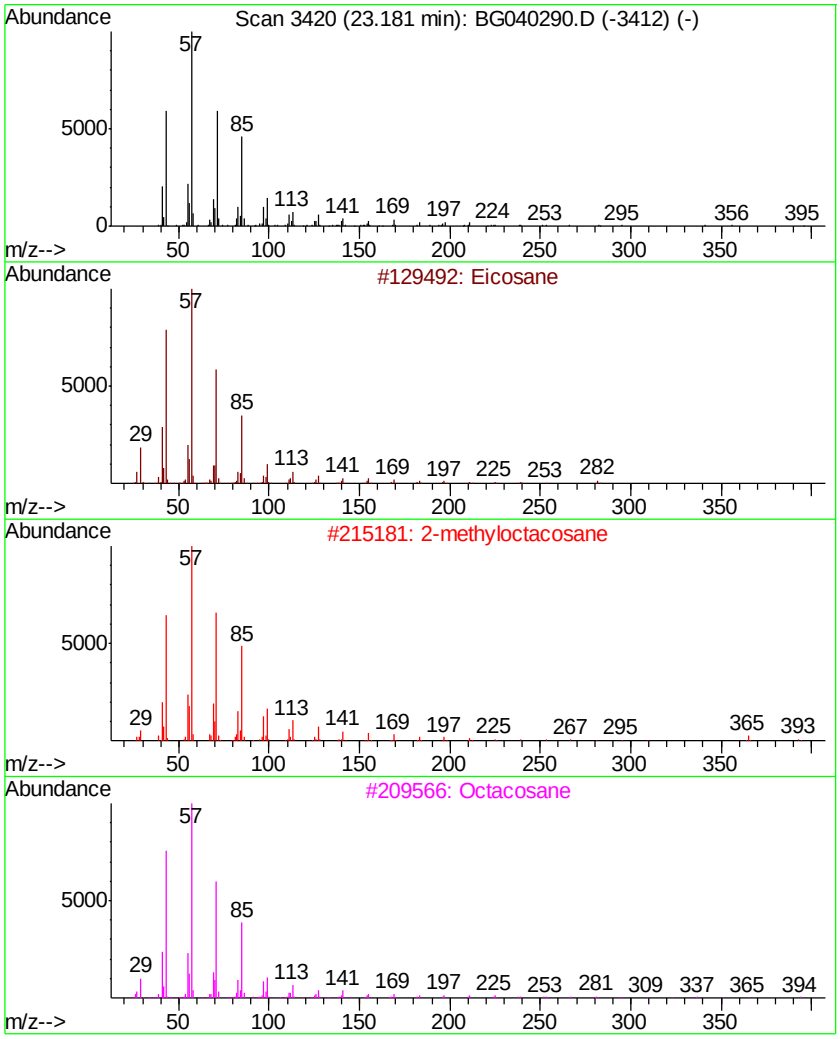
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

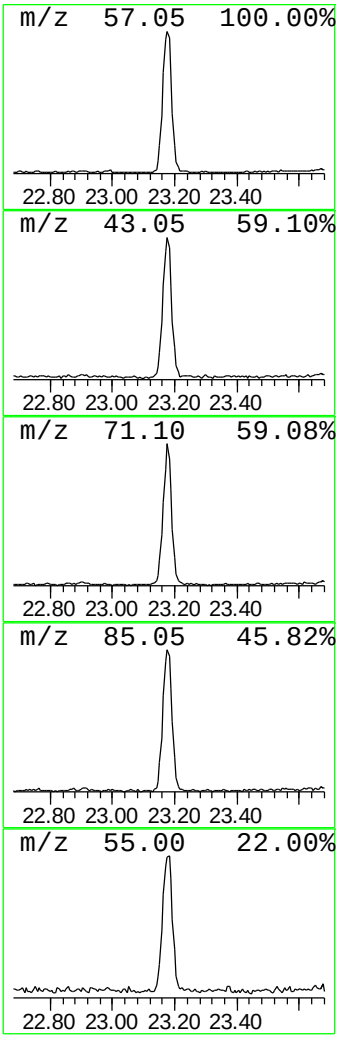
****

Peak Number 7 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.18	8.07 ng	461594	Chrysene-d12	21.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Heptacosane	380	C27H56	000593-49-7	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG040119\
Data File : BG040290.D
Acq On : 2 Apr 2019 8:26
Operator : JU/SJ
Sample : K2180-31
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG032719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

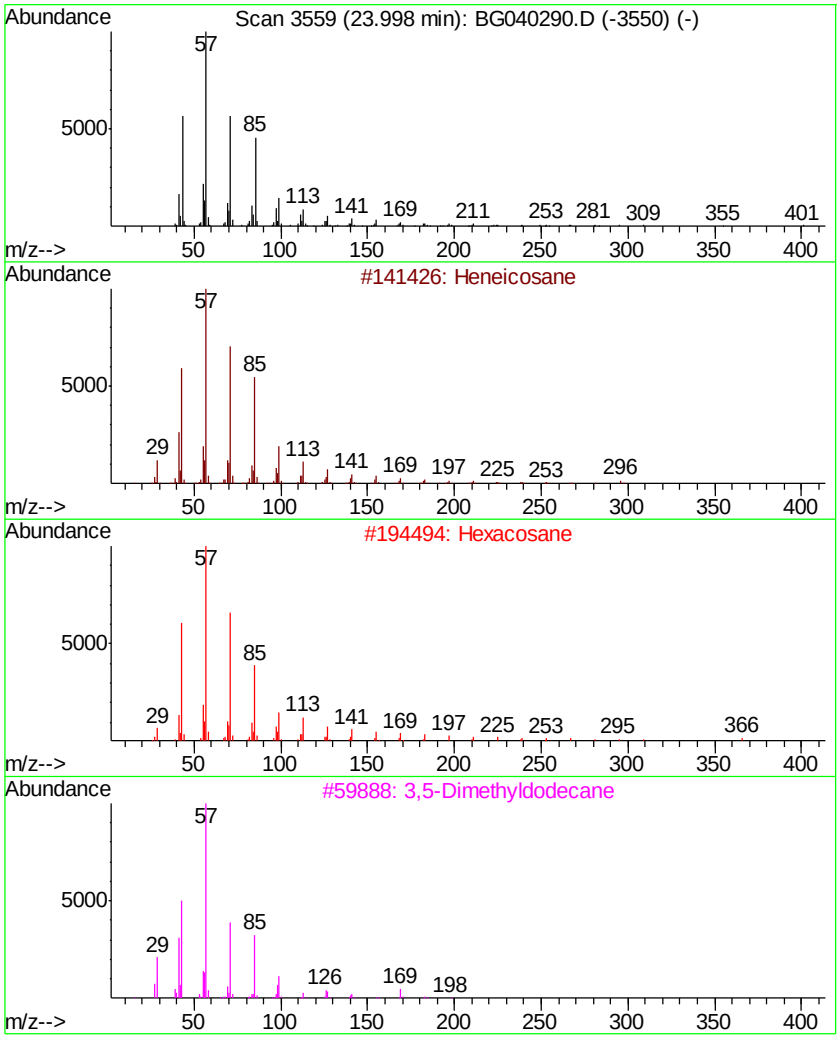
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

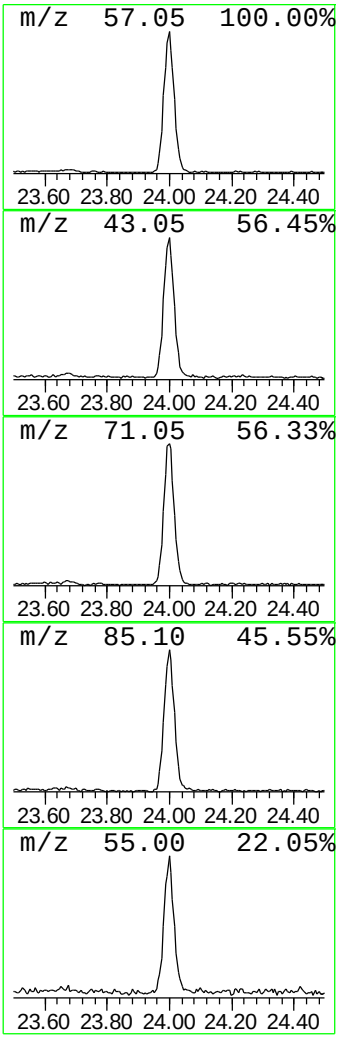
****

Peak Number 8 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.00	6.69 ng	559296	Perylene-d12	25.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Hexacosane	366	C26H54	000630-01-3	90
3	3,5-Dimethyldodecane	198	C14H30	107770-99-0	87
4	Eicosane	282	C20H42	000112-95-8	87
5	Heptadecane	240	C17H36	000629-78-7	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG040119\
Data File : BG040290.D
Acq On : 2 Apr 2019 8:26
Operator : JU/SJ
Sample : K2180-31
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG032719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

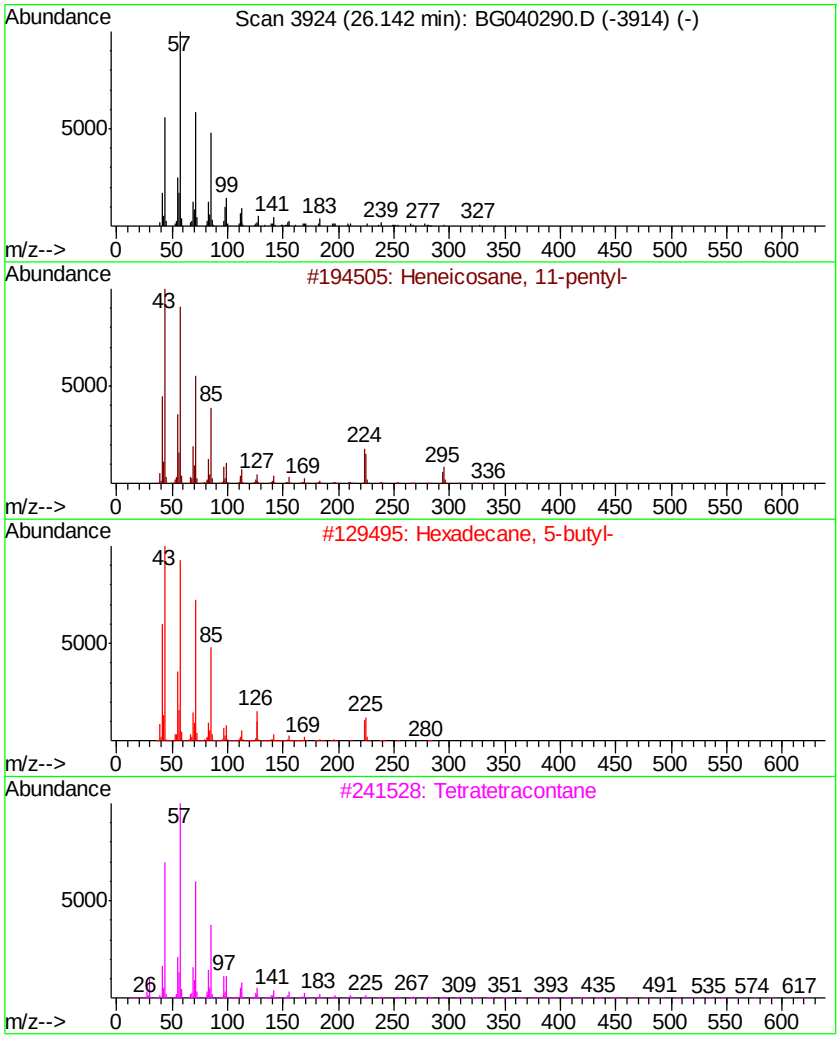
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

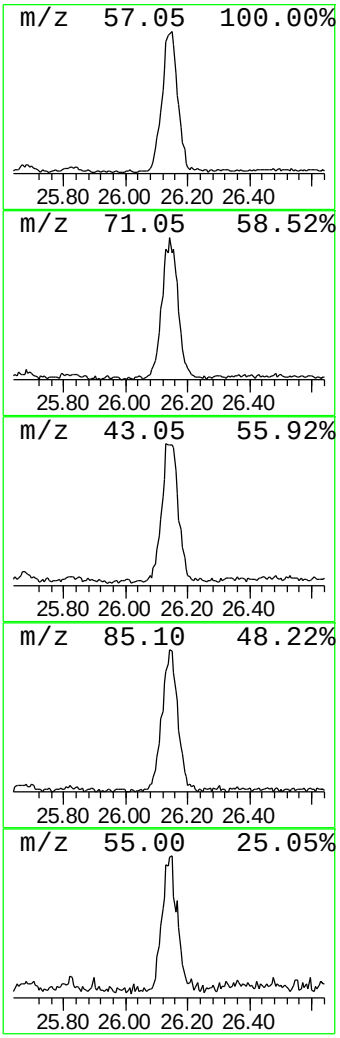
****

Peak Number 9 Heneicosane, 11-pentyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.14	5.12 ng	427769	Perylene-d12	25.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	90
2	Hexadecane, 5-butyl-	282	C20H42	006912-07-8	87
3	Tetratetracontane	619	C44H90	007098-22-8	87
4	2-methyloctacosane	408	C29H60	1000376-72-8	87
5	Tetracosane	338	C24H50	000646-31-1	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG040119\
Data File : BG040290.D
Acq On : 2 Apr 2019 8:26
Operator : JU/SJ
Sample : K2180-31
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG032719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

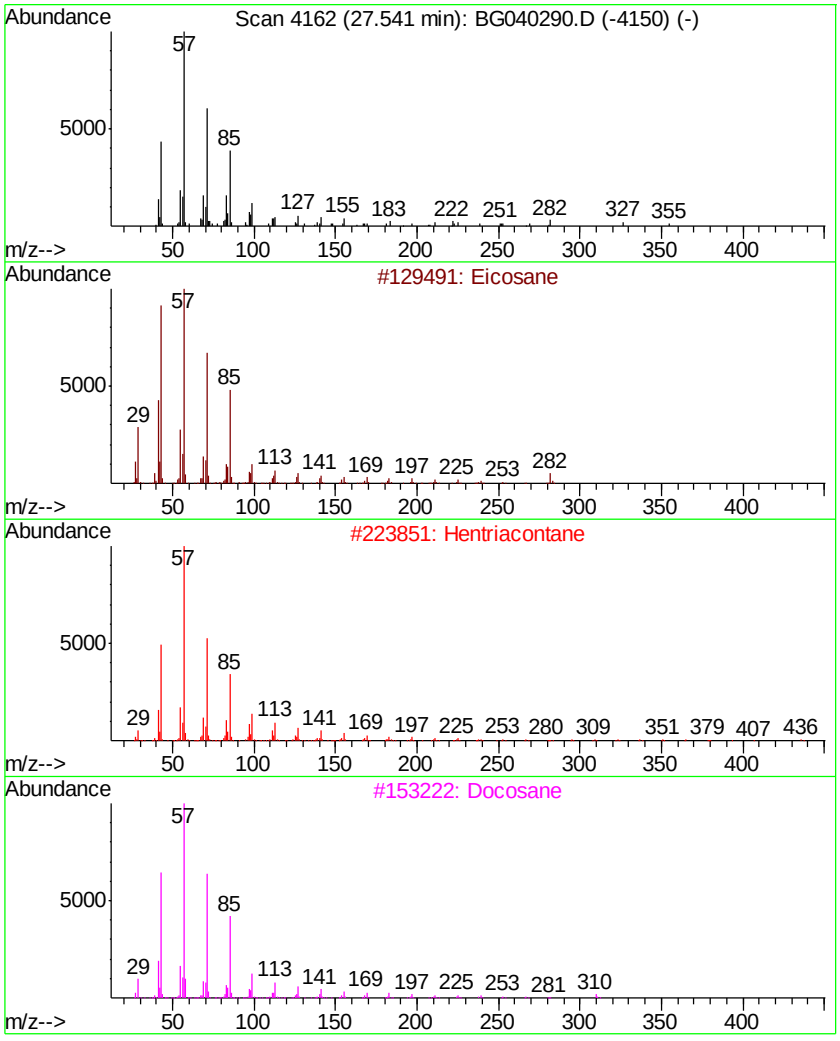
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

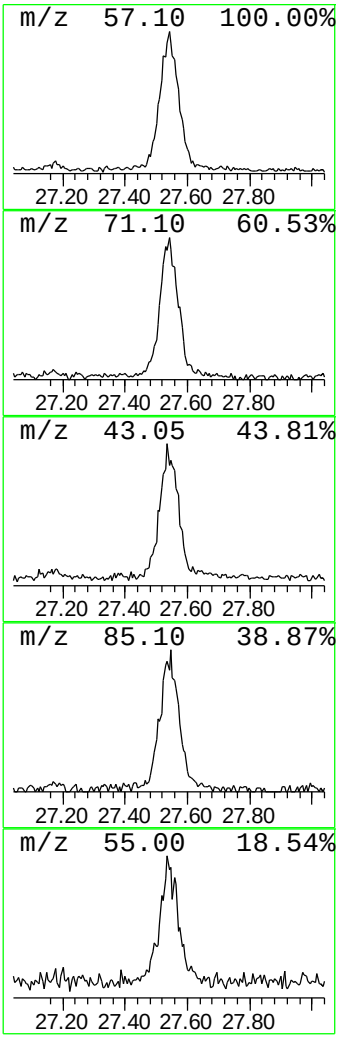
****

Peak Number 10 Hentriacontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.54	3.17 ng	264701	Perylene-d12	25.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Hentriacontane	437	C31H64	000630-04-6	83
3	Docosane	310	C22H46	000629-97-0	83
4	Octacosane	394	C28H58	000630-02-4	83
5	Pentadecane	212	C15H32	000629-62-9	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG040119\
Data File : BG040290.D
Acq On : 2 Apr 2019 8:26
Operator : JU/SJ
Sample : K2180-31
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG032719.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
unknown7.58	7.58	100.9	ng	1659790	1	8.05	328894	20.0
Tetratriacontyl t...	21.31	4.6	ng	264326	5	21.71	1144660	20.0
2-Bromo dodecane	21.85	3.0	ng	168843	5	21.71	1144660	20.0
Octacosane	22.47	5.3	ng	304994	5	21.71	1144660	20.0
Eicosane	23.18	8.1	ng	461594	5	21.71	1144660	20.0
Heneicosane	24.00	6.7	ng	559296	6	25.01	1672600	20.0
Heneicosane, 11-p...	26.14	5.1	ng	427769	6	25.01	1672600	20.0
Hentriacontane	27.54	3.2	ng	264701	6	25.01	1672600	20.0