LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG040119\
Data File : BG040281.D
Acq On : 2 Apr 2019 1:34
Operator : JU/SJ
Sample : K2179-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-4D

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	3.123	3	6	13	rVB	64436	97448	2.23%	0.391%
2	5.608	422	429	442	rVB	1062820	1703044	38.99%	6.832%
3	7.206	693	701	713	rBV	1157441	1987998	45.51%	7.975%
4	7.582	757	765	774	rBV	1087913	1844321	42.22%	7.398%
5	8.052	838	845	855	rBV	193000	333585	7.64%	1.338%
6	8.375	892	900	910	rVB	761712	1297096	29.69%	5.203%
7	9.227	1037	1045	1055	rBV	652703	1161933	26.60%	4.661%
8	10.867	1317	1324	1332	rBV	273866	498719	11.42%	2.001%
9	13.305	1732	1739	1748	rVB	1844346	2894686	66.27%	11.612%
10	14.128	1873	1879	1886	rBV	120438	173269	3.97%	0.695%
11	14.686	1967	1974	1983	rVB2	501507	803884	18.40%	3.225%
12	16.172	2220	2227	2242	rBV	1707231	2588596	59.26%	10.384%
13	17.430	2435	2441	2448	rBV	717932	1073009	24.56%	4.304%
14	18.287	2582	2587	2591	rBV3	32643	50981	1.17%	0.205%
15	20.032	2878	2884	2892	rBV	3266603	4368293	100.00%	17.523%
16	21.307	3097	3101	3115	rBV4	45465	115436	2.64%	0.463%
17	21.707	3162	3169	3178	rVB	695240	1195400	27.37%	4.795%
18	21.854	3189	3194	3199	rBV2	66404	94822	2.17%	0.380%
19	22.471	3293	3299	3305	rBV	110718	184944	4.23%	0.742%
20	23.176	3412	3419	3427	rBV2	140752	266874	6.11%	1.071%
21	23.992	3549	3558	3569	rBV2	148188	336559	7.70%	1.350%
22	25.009	3714	3731	3747	rBV4	359916	1484989	33.99%	5.957%
23	26.131	3912	3922	3934	rBV3	72951	250793	5.74%	1.006%
24	27.529	4151	4160	4170	rVB5	34708	122012	2.79%	0.489%

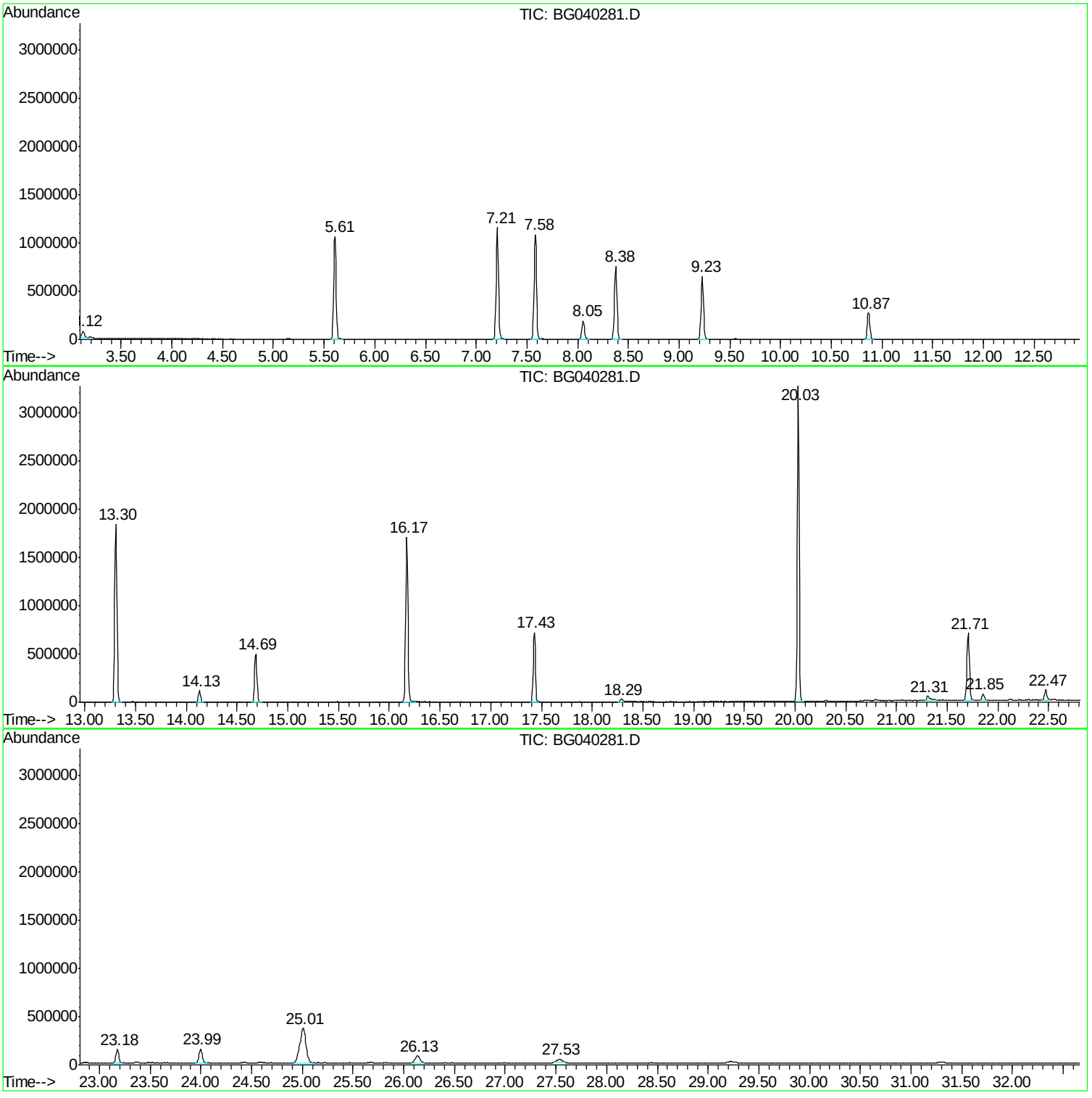
Sum of corrected areas: 24928691

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG040119\
Data File : BG040281.D
Acq On : 2 Apr 2019 1:34
Operator : JU/SJ
Sample : K2179-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-4D

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 : BG040281.D
Acq On : 2 Apr 2019 1:34
Operator : JU/SJ
Sample : K2179-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-4D

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

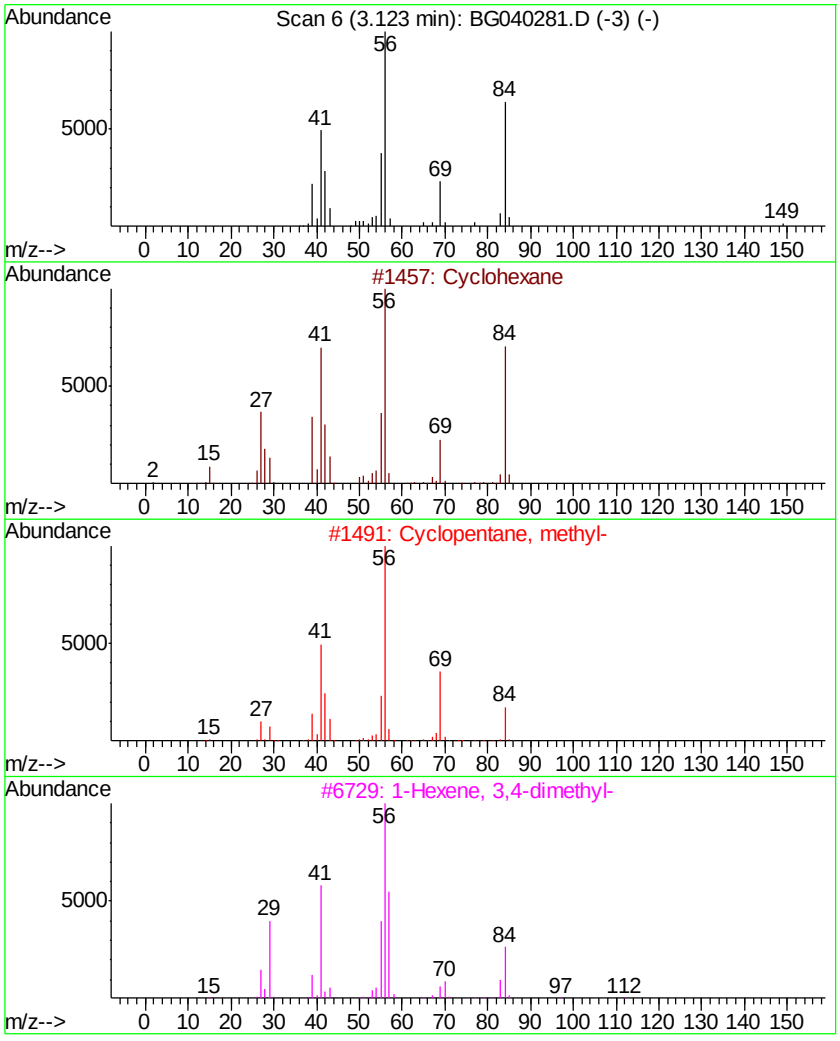
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

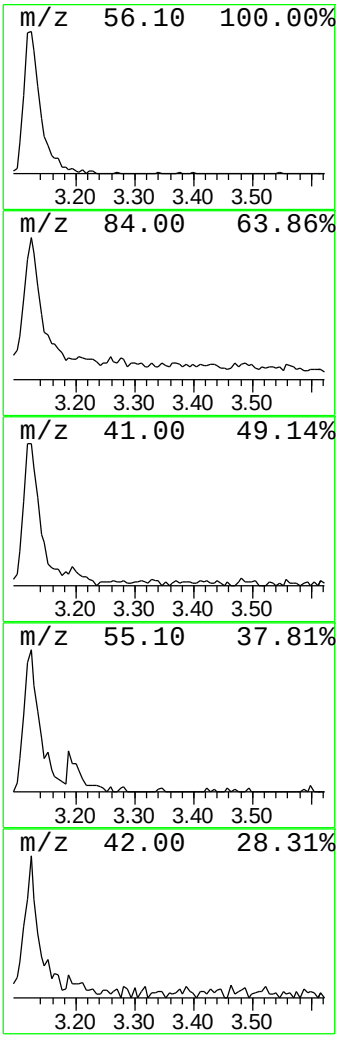
****

Peak Number 1 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.12	5.84 ng	97448	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane	84	C6H12	000110-82-7	91
2	Cyclopentane, methyl-	84	C6H12	000096-37-7	72
3	1-Hexene, 3,4-dimethyl-	112	C8H16	016745-94-1	64
4	2-Amino-oxazole	84	C3H4N2O	004570-45-0	64
5	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	50





Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG040119\
Data File : BG040281.D
Acq On : 2 Apr 2019 1:34
Operator : JU/SJ
Sample : K2179-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-4D

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

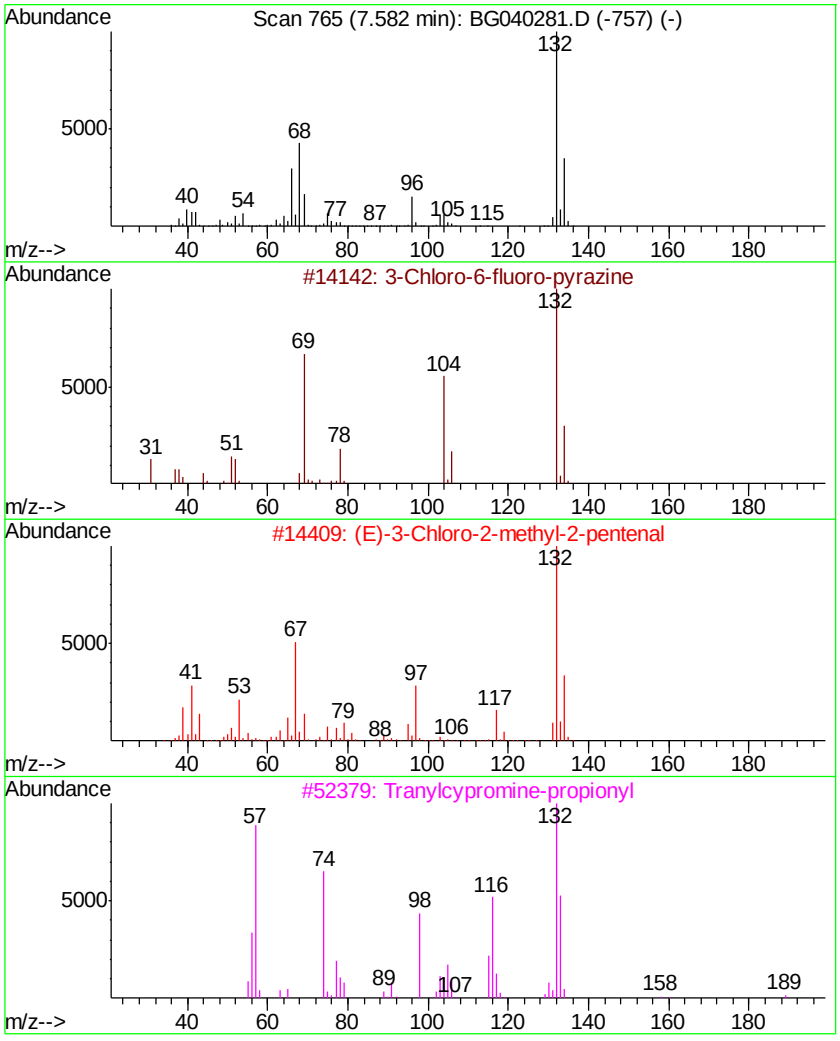
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

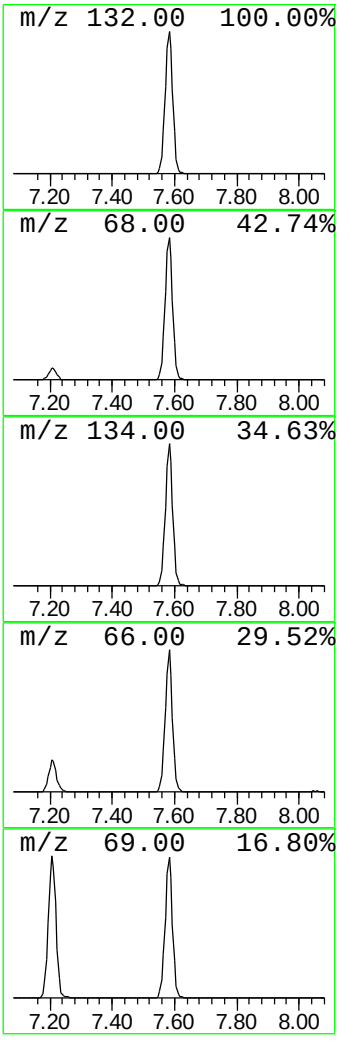
****

Peak Number 2 unknown7.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	110.58 ng	1844320	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10





Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG040119\
Data File : BG040281.D
Acq On : 2 Apr 2019 1:34
Operator : JU/SJ
Sample : K2179-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-4D

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

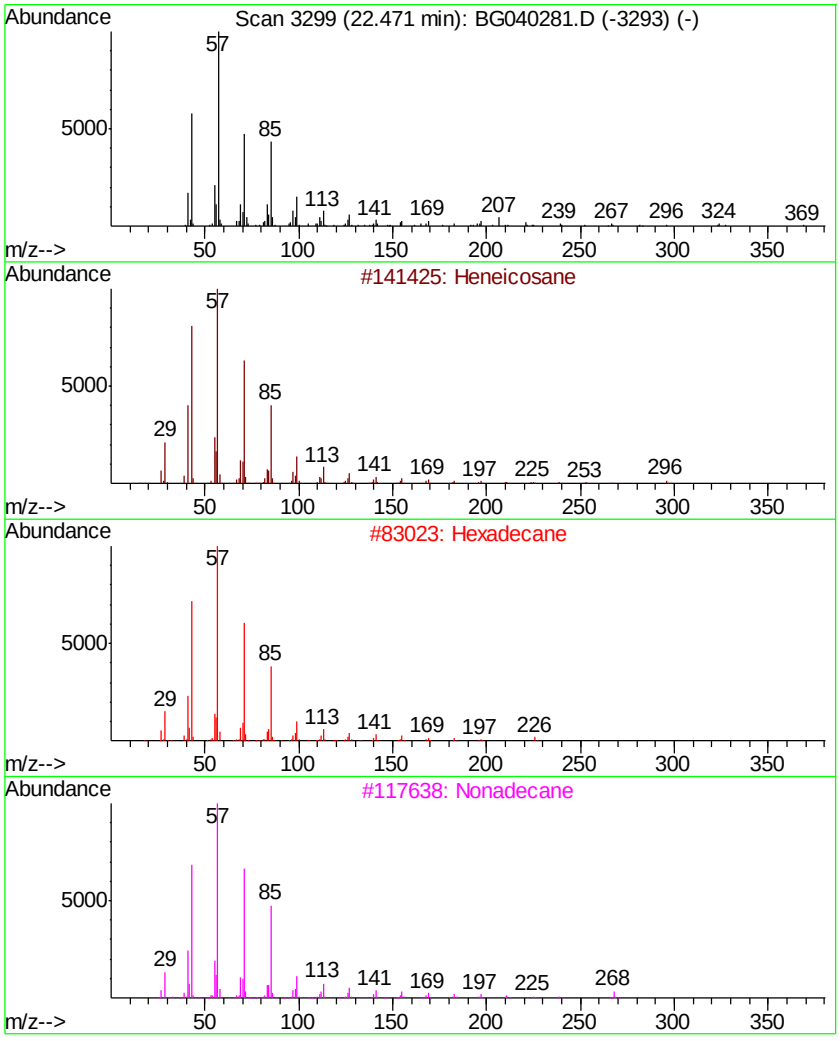
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

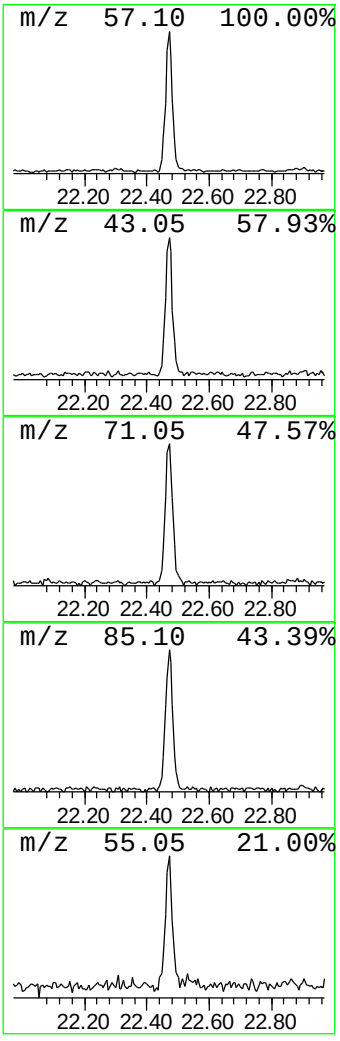
****

Peak Number 4 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.47	3.09 ng	184944	Chrysene-d12	21.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hexadecane	226	C16H34	000544-76-3	87
3	Nonadecane	268	C19H40	000629-92-5	87
4	Heptadecane	240	C17H36	000629-78-7	86
5	1-Iodoundecane	282	C11H23I	004282-44-4	83





Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG040119\
Data File : BG040281.D
Acq On : 2 Apr 2019 1:34
Operator : JU/SJ
Sample : K2179-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-4D

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

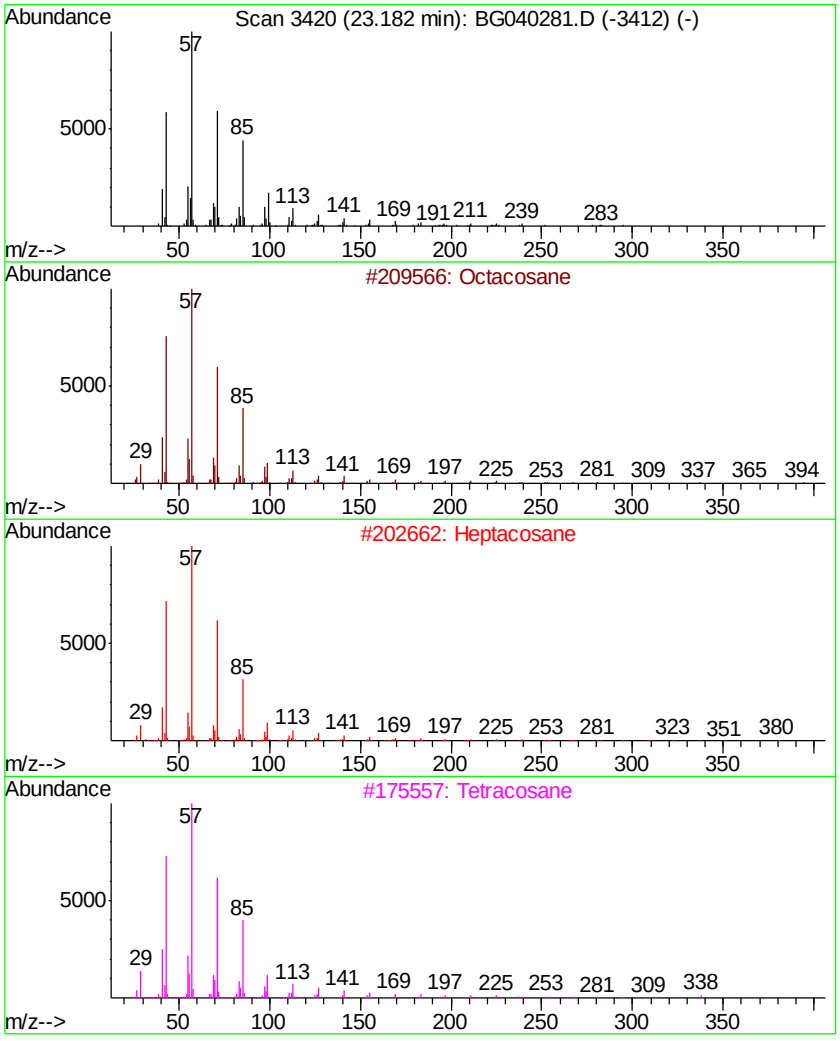
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

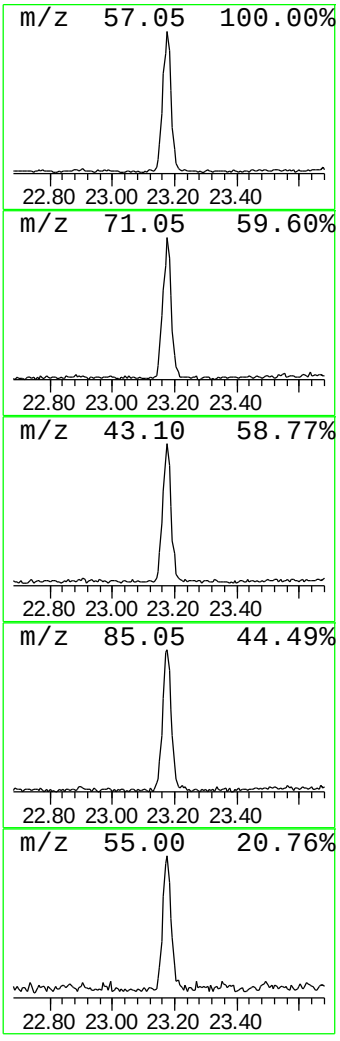
****

Peak Number 5 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.18	4.47 ng	266874	Chrysene-d12	21.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heptacosane	380	C27H56	000593-49-7	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Hexacosane	366	C26H54	000630-01-3	90
5	Triacontane	422	C30H62	000638-68-6	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG040119\
Data File : BG040281.D
Acq On : 2 Apr 2019 1:34
Operator : JU/SJ
Sample : K2179-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-4D

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

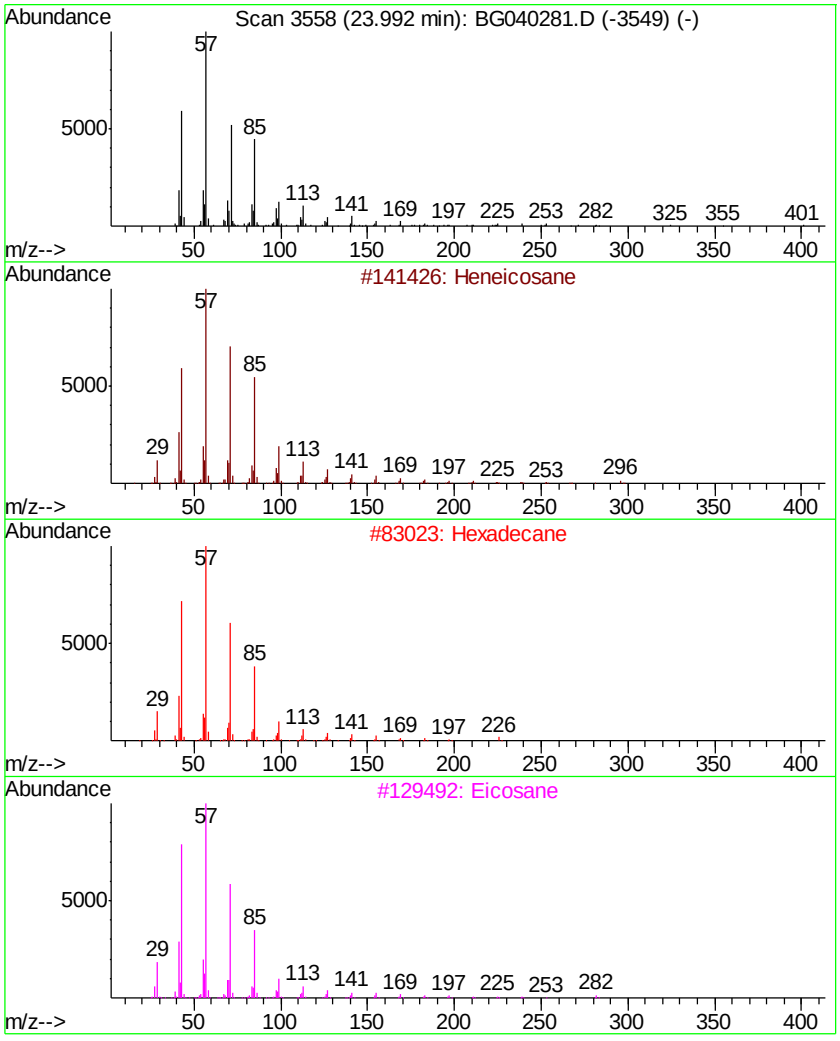
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

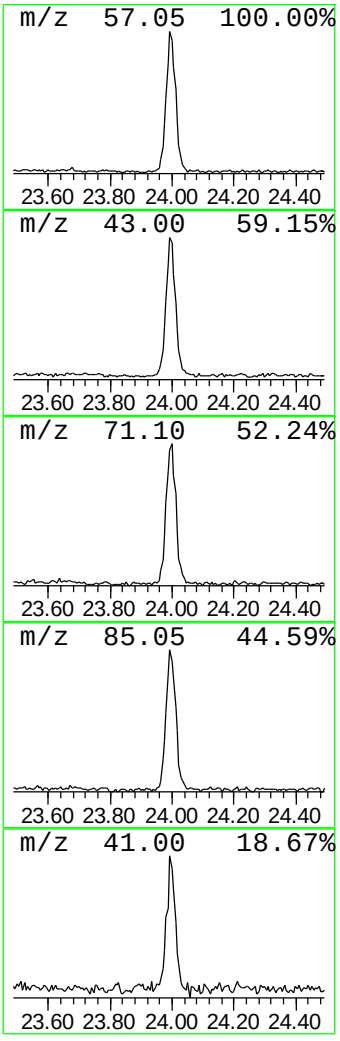
****

Peak Number 6 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.99	4.53 ng	336559	Perylene-d12	25.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Hexadecane	226	C16H34	000544-76-3	87
3	Eicosane	282	C20H42	000112-95-8	86
4	Octadecane	254	C18H38	000593-45-3	83
5	Octacosane	394	C28H58	000630-02-4	81





Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG040119\
Data File : BG040281.D
Acq On : 2 Apr 2019 1:34
Operator : JU/SJ
Sample : K2179-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-4D

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

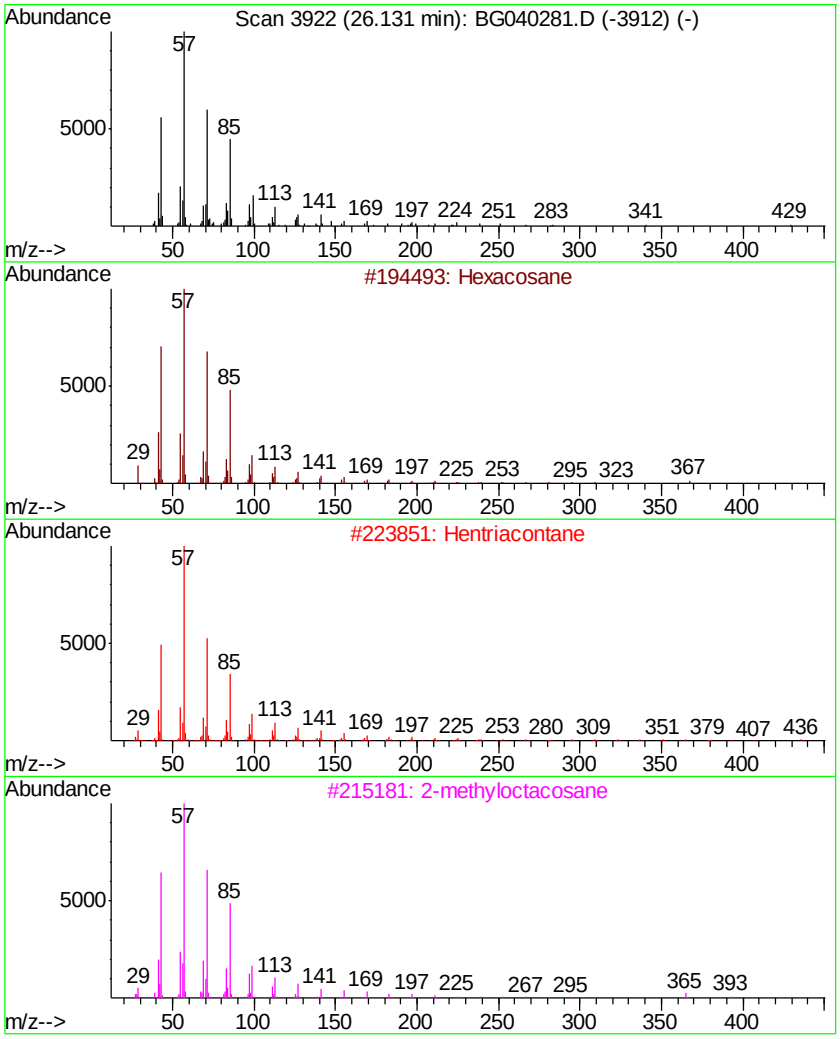
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

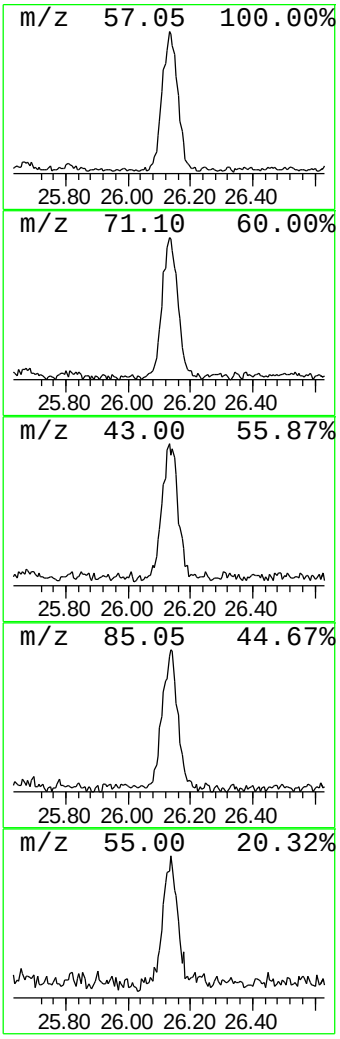
****

Peak Number 7 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.13	3.38 ng	250793	Perylene-d12	25.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	90
2	Hentriacontane	437	C31H64	000630-04-6	90
3	2-methyloctacosane	408	C29H60	1000376-72-8	90
4	Tetracosane	338	C24H50	000646-31-1	87
5	Pentacosane	352	C25H52	000629-99-2	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG040119\
Data File : BG040281.D
Acq On : 2 Apr 2019 1:34
Operator : JU/SJ
Sample : K2179-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-4D

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
Cyclopentane, met...	3.12	5.8	ng	97448	1	8.05	333585	20.0
unknown7.58	7.58	110.6	ng	1844320	1	8.05	333585	20.0
Heneicosane	22.47	3.1	ng	184944	5	21.71	1195400	20.0
Octacosane	23.18	4.5	ng	266874	5	21.71	1195400	20.0
Eicosane	23.99	4.5	ng	336559	6	25.01	1484990	20.0
Hexacosane	26.13	3.4	ng	250793	6	25.01	1484990	20.0