LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG040119\
Data File : BG040280.D
Acq On : 2 Apr 2019 00:55
Operator : JU/SJ
Sample : K2179-15
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-8D

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	16	rVB	166587	269400	10.55%	1.615%
2	3.199	16	19	27	rVB4	15808	27400	1.07%	0.164%
3	5.143	345	350	359	rVB	27026	42426	1.66%	0.254%
4	5.607	422	429	437	rBV	574776	910436	35.66%	5.457%
5	7.206	693	701	710	rBV	633890	1073205	42.03%	6.433%
6	7.582	756	765	774	rBV	588752	1005724	39.39%	6.029%
7	8.052	839	845	857	rVB	200400	337399	13.21%	2.022%
8	8.375	892	900	909	rVB	406345	697671	27.32%	4.182%
9	9.227	1034	1045	1055	rBV	346401	620389	24.30%	3.719%
10	10.866	1317	1324	1333	rBV	290129	514613	20.15%	3.085%
11	13.304	1732	1739	1747	rBV	1057410	1597375	62.56%	9.575%
12	14.127	1873	1879	1885	rBV	53045	78801	3.09%	0.472%
13	14.685	1967	1974	1983	rVB2	530555	841620	32.96%	5.045%
14	16.172	2220	2227	2238	rBV	930905	1390644	54.46%	8.336%
15	17.429	2433	2441	2448	rBV2	739806	1128854	44.21%	6.767%
16	18.287	2582	2587	2596	rBV3	24170	47347	1.85%	0.284%
17	20.026	2878	2883	2891	rBV	1820430	2553343	100.00%	15.305%
18	21.307	3095	3101	3110	rBV2	73616	187340	7.34%	1.123%
19	21.706	3162	3169	3181	rVB2	749028	1246920	48.83%	7.474%
20	21.853	3190	3194	3200	rVB3	34202	49254	1.93%	0.295%
21	22.470	3294	3299	3306	rVB2	54723	87634	3.43%	0.525%
22	23.169	3413	3418	3425	rVB3	72970	145917	5.71%	0.875%
23	23.998	3551	3559	3567	rVB3	85436	192506	7.54%	1.154%
24	25.008	3715	3731	3746	rVB2	414414	1397308	54.72%	8.376%
25	26.131	3913	3922	3935	rVB3	45616	163880	6.42%	0.982%
26	27.523	4151	4159	4169	rVB5	24533	75227	2.95%	0.451%

Sum of corrected areas: 16682633

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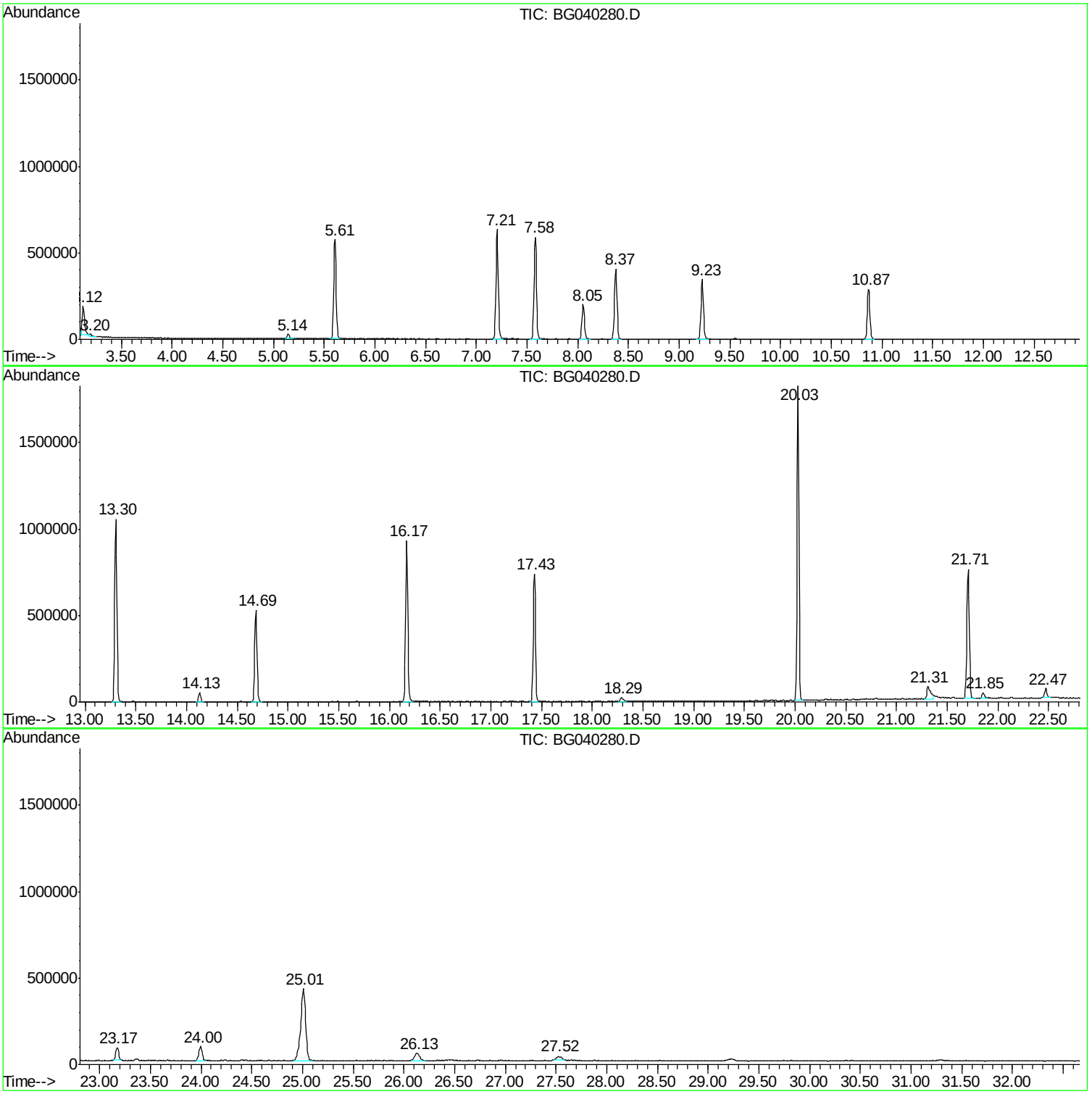
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-8D

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



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Data File : BG040280.D
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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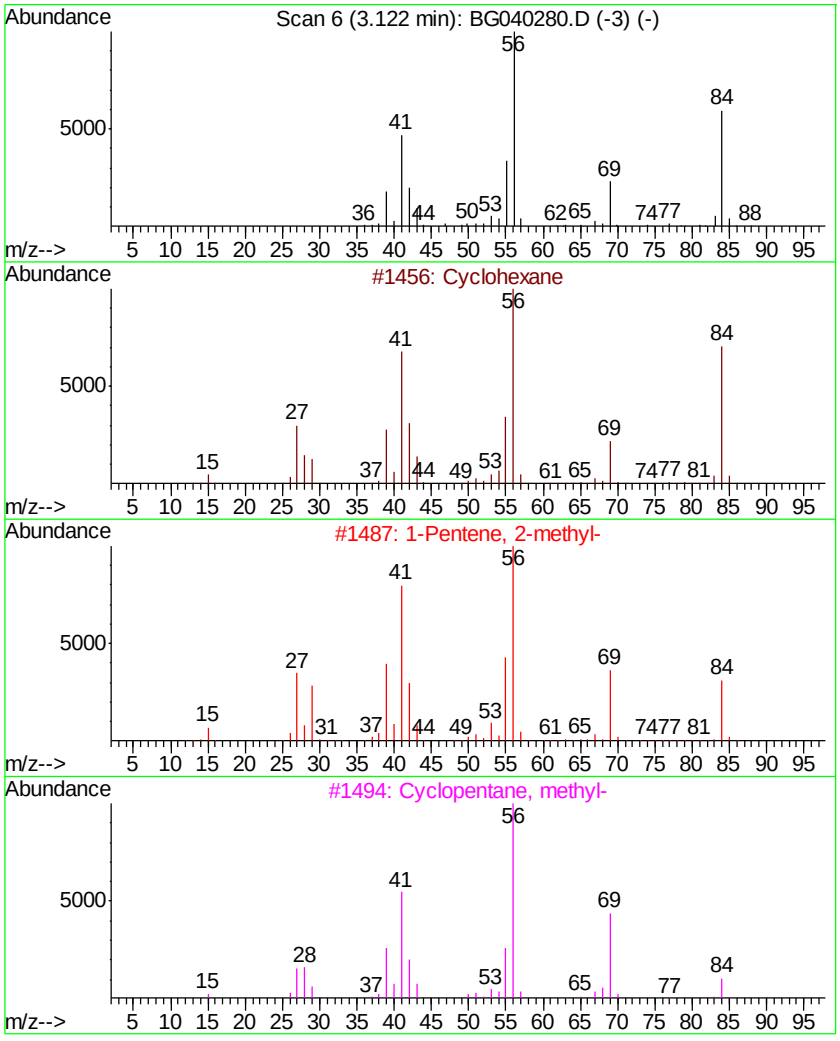
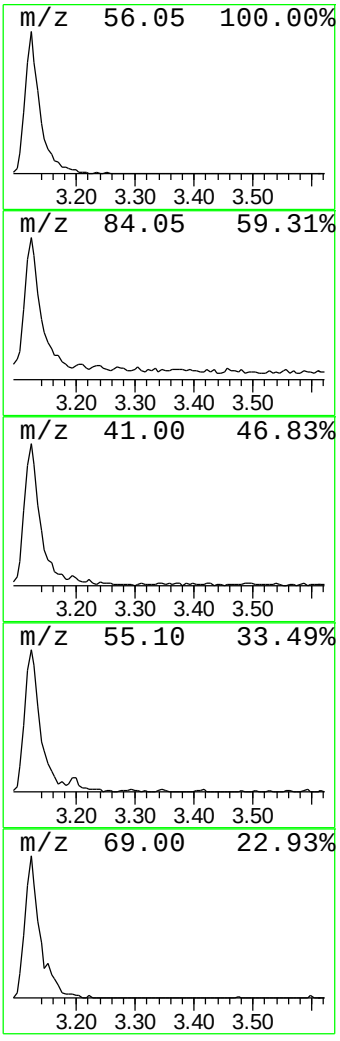
Peak Number 1 1-Pentene, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.12	15.97 ng	269400	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane	84	C6H12	000110-82-7	91
2	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	64
3	Cyclopentane, methyl-	84	C6H12	000096-37-7	42
4	2-Amino-oxazole	84	C3H4N2O	004570-45-0	38
5	Cyclobutane, ethyl-	84	C6H12	004806-61-5	38





Library Search Compound Report

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Data File : BG040280.D
Acq On : 2 Apr 2019 00:55
Operator : JU/SJ
Sample : K2179-15
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-8D

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

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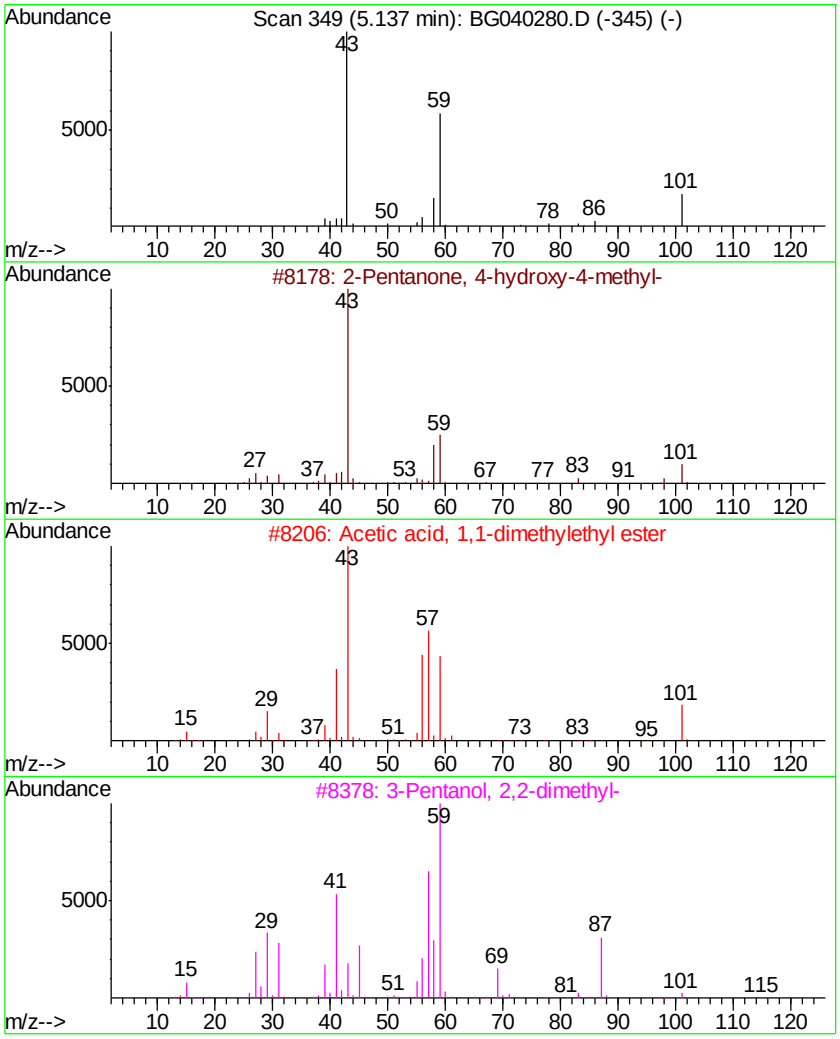
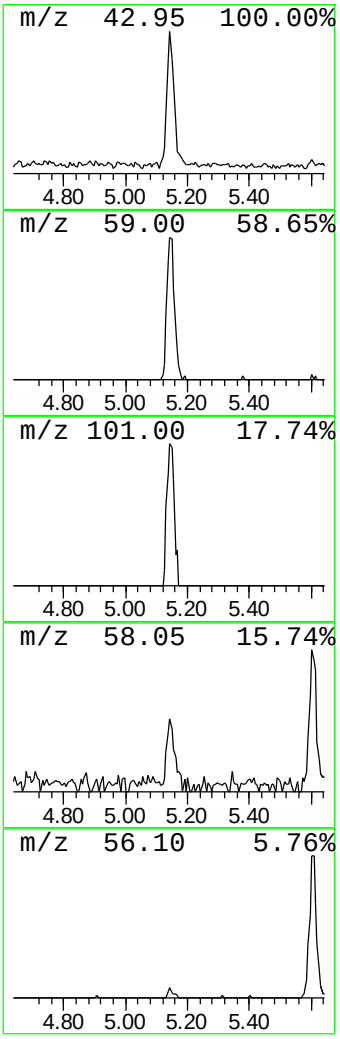
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	2.51 ng	42426	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	33
4	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	10





Library Search Compound Report

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Data File : BG040280.D
Acq On : 2 Apr 2019 00:55
Operator : JU/SJ
Sample : K2179-15
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-8D

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
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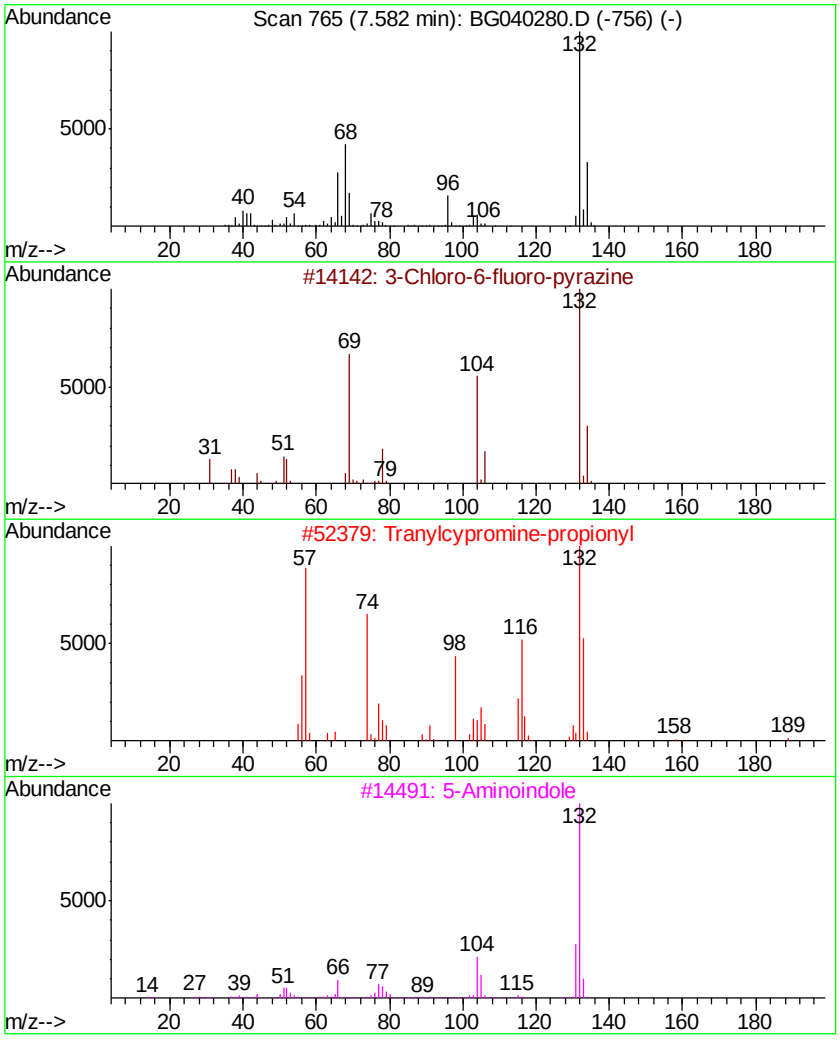
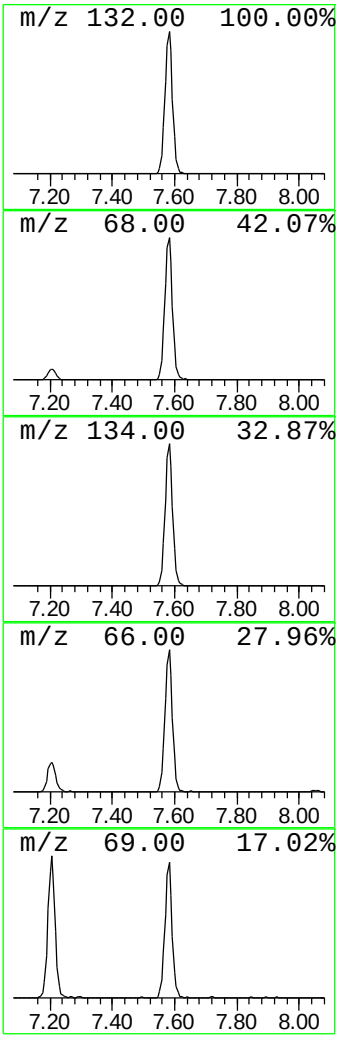
Peak Number 3 unknown7.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	59.62 ng	1005720	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	16
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Xenon	132	Xe	007440-63-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG040119\
Data File : BG040280.D
Acq On : 2 Apr 2019 00:55
Operator : JU/SJ
Sample : K2179-15
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-8D

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

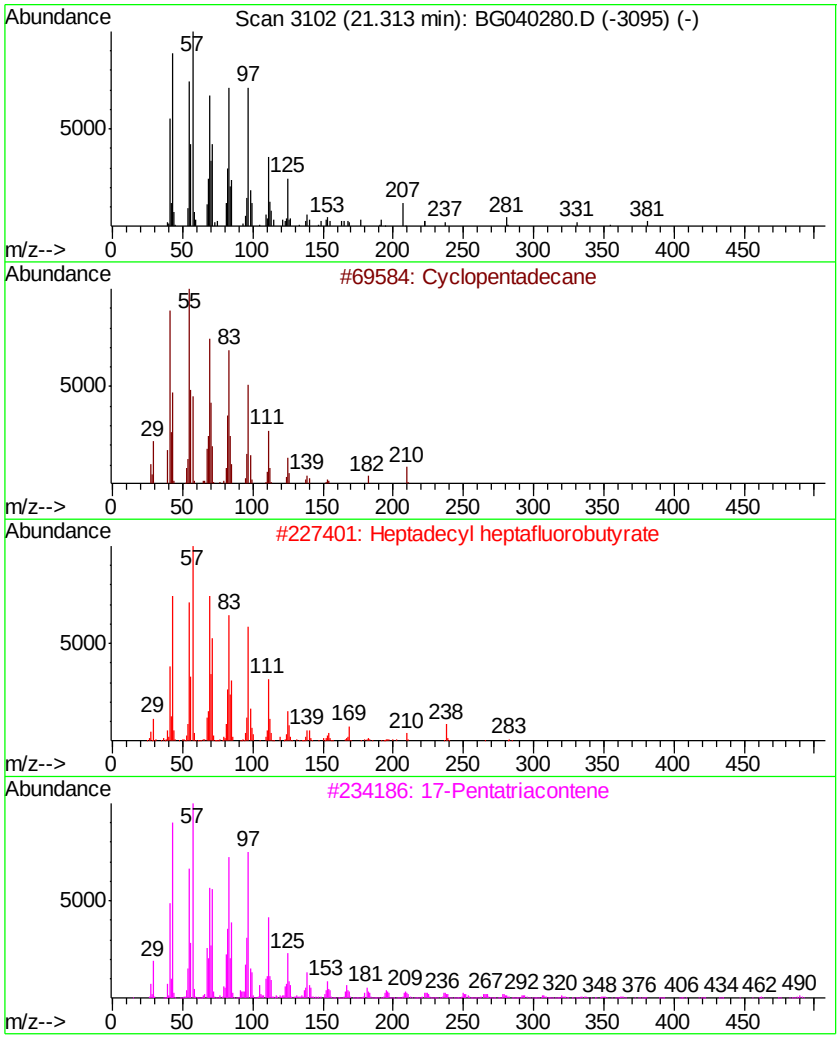
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

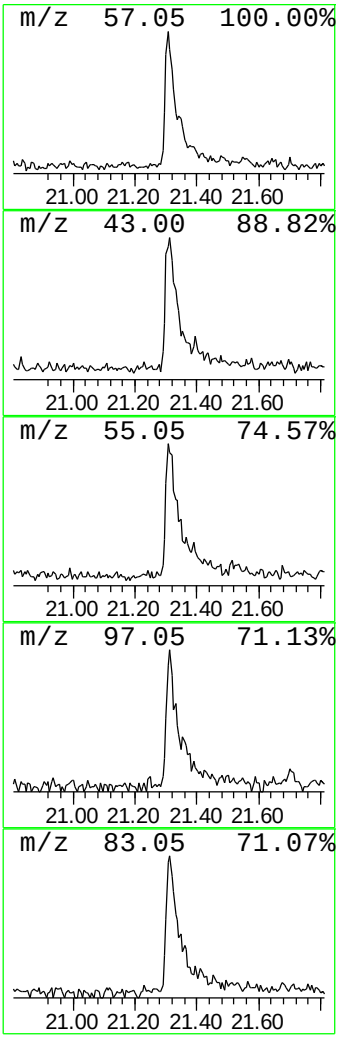
****

Peak Number 5 Cyclopentadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.31	3.00 ng	187340	Chrysene-d12	21.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	97
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90
3	17-Pentatriacontene	491	C35H70	006971-40-0	87
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	81
5	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	81





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG040119\
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Operator : JU/SJ
Sample : K2179-15
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-8D

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

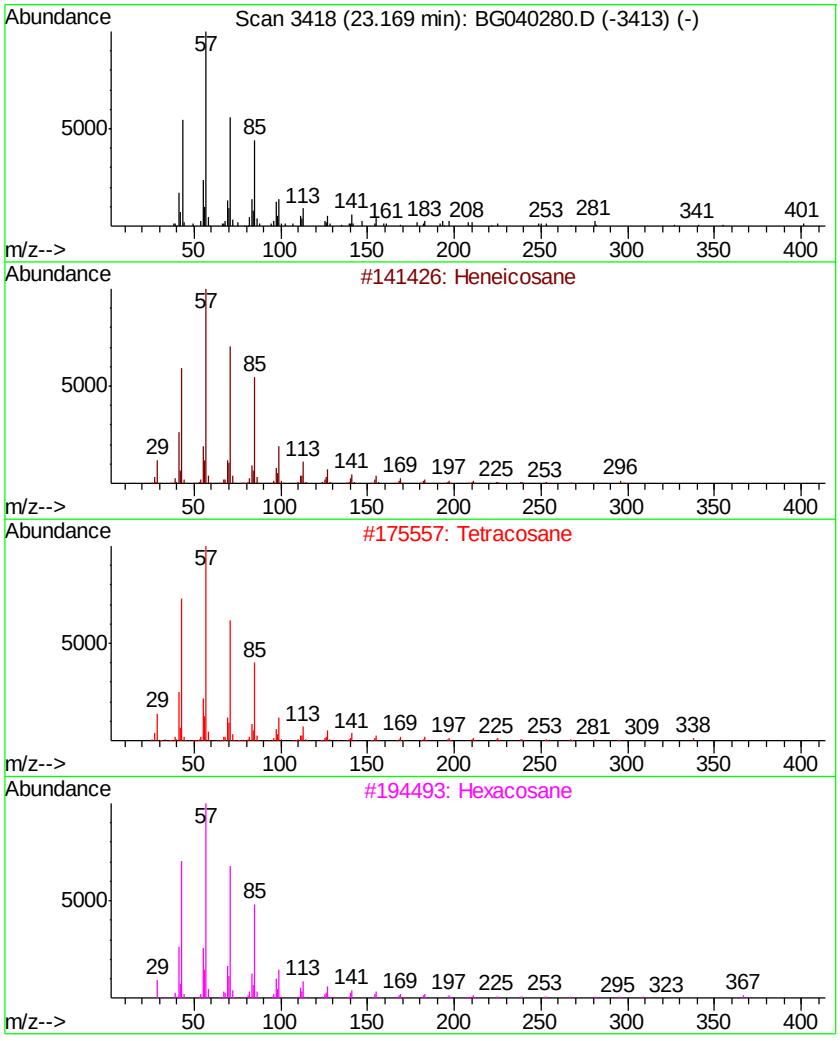
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

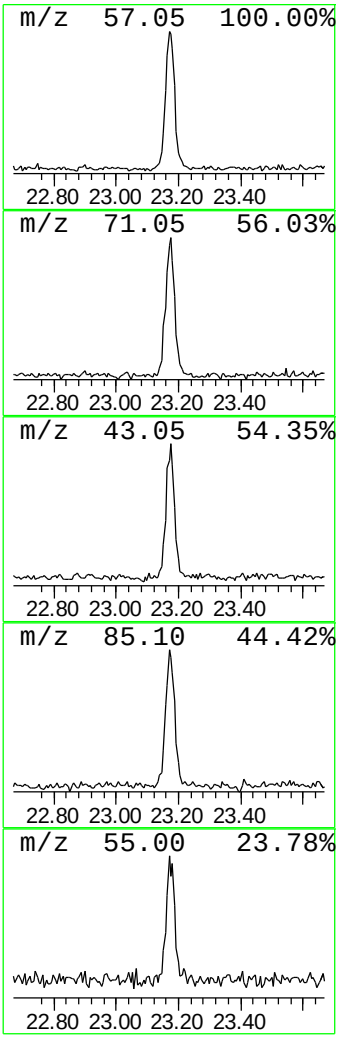
****

Peak Number 6 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.17	2.34 ng	145917	Chrysene-d12	21.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Tetracosane	338	C24H50	000646-31-1	90
3	Hexacosane	366	C26H54	000630-01-3	90
4	Octacosane	394	C28H58	000630-02-4	87
5	Pentacosane	352	C25H52	000629-99-2	87





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Operator : JU/SJ
Sample : K2179-15
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-8D

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
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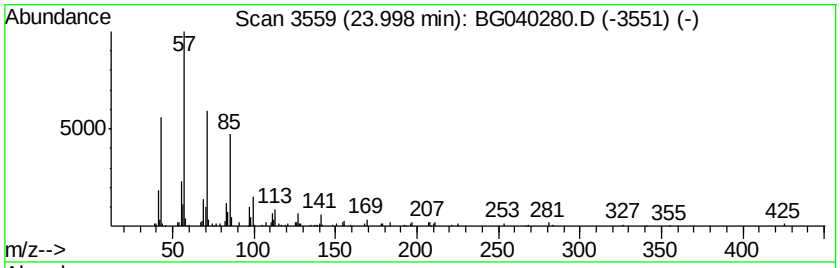
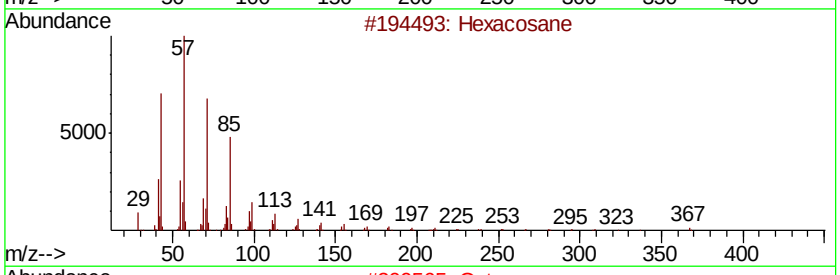
****

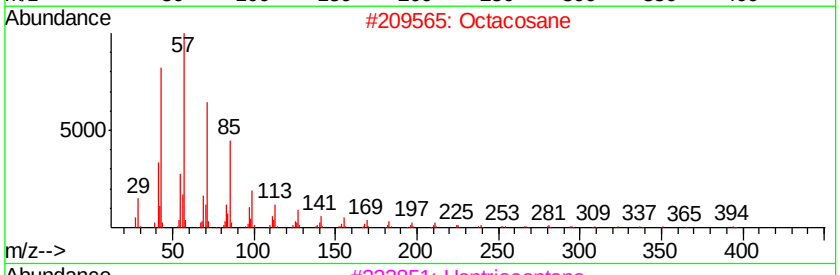
Peak Number 7 Hexacosane Concentration Rank 5

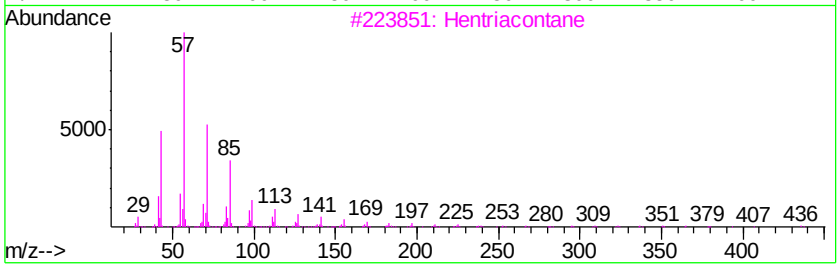
R.T.	EstConc	Area	Relative to ISTD	R.T.
24.00	2.76 ng	192506	Perylene-d12	25.01

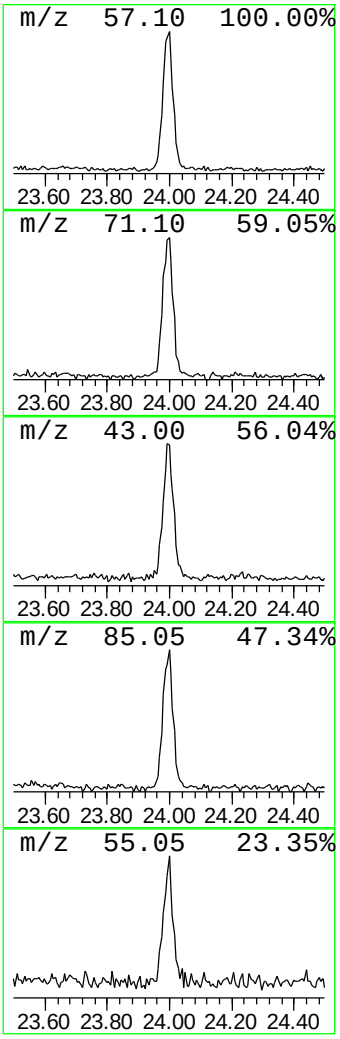
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	93
2	Octacosane	394	C28H58	000630-02-4	91
3	Hentriacontane	437	C31H64	000630-04-6	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	Tetratetracontane	619	C44H90	007098-22-8	90











Library Search Compound Report

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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-8D

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

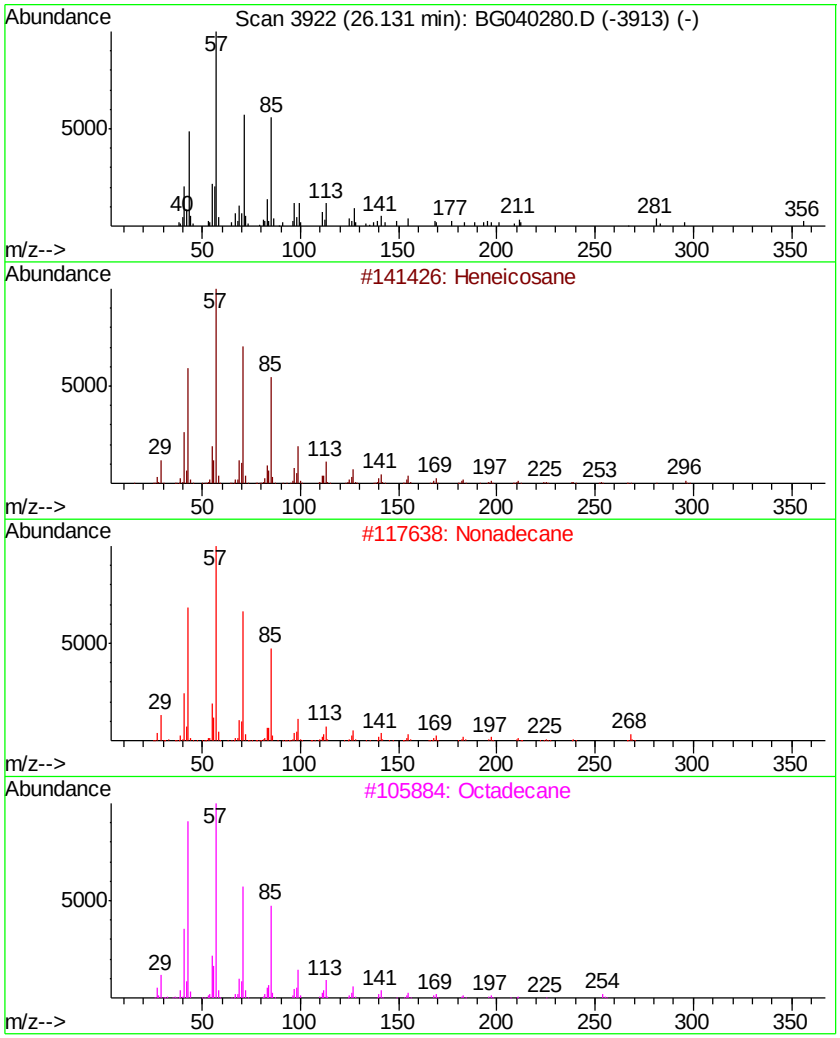
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

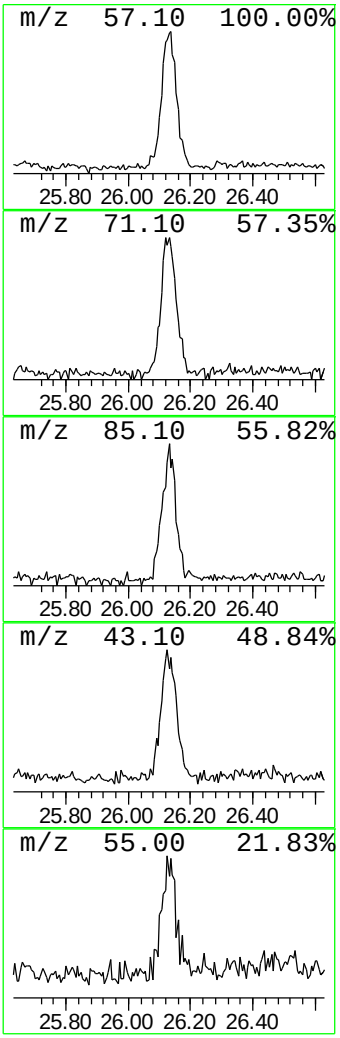
****

Peak Number 8 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.13	2.35 ng	163880	Perylene-d12	25.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	93
2	Nonadecane	268	C19H40	000629-92-5	80
3	Octadecane	254	C18H38	000593-45-3	80
4	Hexacosane	366	C26H54	000630-01-3	72
5	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	72





Tentatively Identified Compound (LSC) summary

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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	16.0	ng	269400	1	8.05	337399	20.0
2-Pentanone, 4-hy...	5.14	2.5	ng	42426	1	8.05	337399	20.0
unknown7.58	7.58	59.6	ng	1005720	1	8.05	337399	20.0
Cyclopentadecane	21.31	3.0	ng	187340	5	21.71	1246920	20.0
Heneicosane	23.17	2.3	ng	145917	5	21.71	1246920	20.0
Hexacosane	24.00	2.8	ng	192506	6	25.01	1397310	20.0
Nonadecane	26.13	2.4	ng	163880	6	25.01	1397310	20.0