LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG100719\
Data File : BG043076.D
Acq On : 7 Oct 2019 20:27
Operator : JU
Sample : K5154-24
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-101S

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-BG092519.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	3.167	7	13	21	rBV	168104	331560	5.93%	1.315%
2	3.244	21	26	45	rVB	529692	814469	14.56%	3.231%
3	4.783	283	288	296	rVB2	42892	70024	1.25%	0.278%
4	5.641	426	434	446	rBV	574908	965760	17.27%	3.831%
5	7.227	696	704	716	rBV	402783	766002	13.70%	3.038%
6	7.598	758	767	780	rBV	953198	1671844	29.89%	6.631%
7	8.056	837	845	855	rBV	188464	325448	5.82%	1.291%
8	8.379	892	900	909	rBV	673670	1219373	21.80%	4.837%
9	9.219	1035	1043	1053	rBV	578220	1073169	19.19%	4.257%
10	10.858	1315	1322	1333	rBV	236888	438680	7.84%	1.740%
11	13.303	1730	1738	1749	rBV	1806281	2824422	50.50%	11.203%
12	14.125	1872	1878	1889	rVB	154202	227677	4.07%	0.903%
13	14.677	1965	1972	1980	rBV	474948	727236	13.00%	2.885%
14	16.164	2216	2225	2235	rBV	1880325	2956690	52.87%	11.728%
15	17.421	2432	2439	2448	rBV2	643810	985585	17.62%	3.909%
16	18.314	2584	2591	2606	rBV3	207313	485874	8.69%	1.927%
17	19.584	2801	2807	2824	rBV2	172985	447837	8.01%	1.776%
18	20.030	2876	2883	2892	rBV	4134466	5592582	100.00%	22.183%
19	20.829	3013	3019	3023	rBV2	67174	100071	1.79%	0.397%
20	21.334	3101	3105	3110	rBV	68069	84945	1.52%	0.337%
21	21.687	3159	3165	3177	rVB	691191	1155046	20.65%	4.582%
22	21.881	3194	3198	3204	rVB	89001	129897	2.32%	0.515%
23	22.492	3296	3302	3306	rBV2	89016	152719	2.73%	0.606%
24	23.185	3415	3420	3426	rVB2	77395	139254	2.49%	0.552%
25	23.984	3551	3556	3563	rVB	67166	130271	2.33%	0.517%
26	24.907	3702	3713	3727	rVB	418907	1303618	23.31%	5.171%
27	26.064	3905	3910	3918	rVB5	34917	90691	1.62%	0.360%

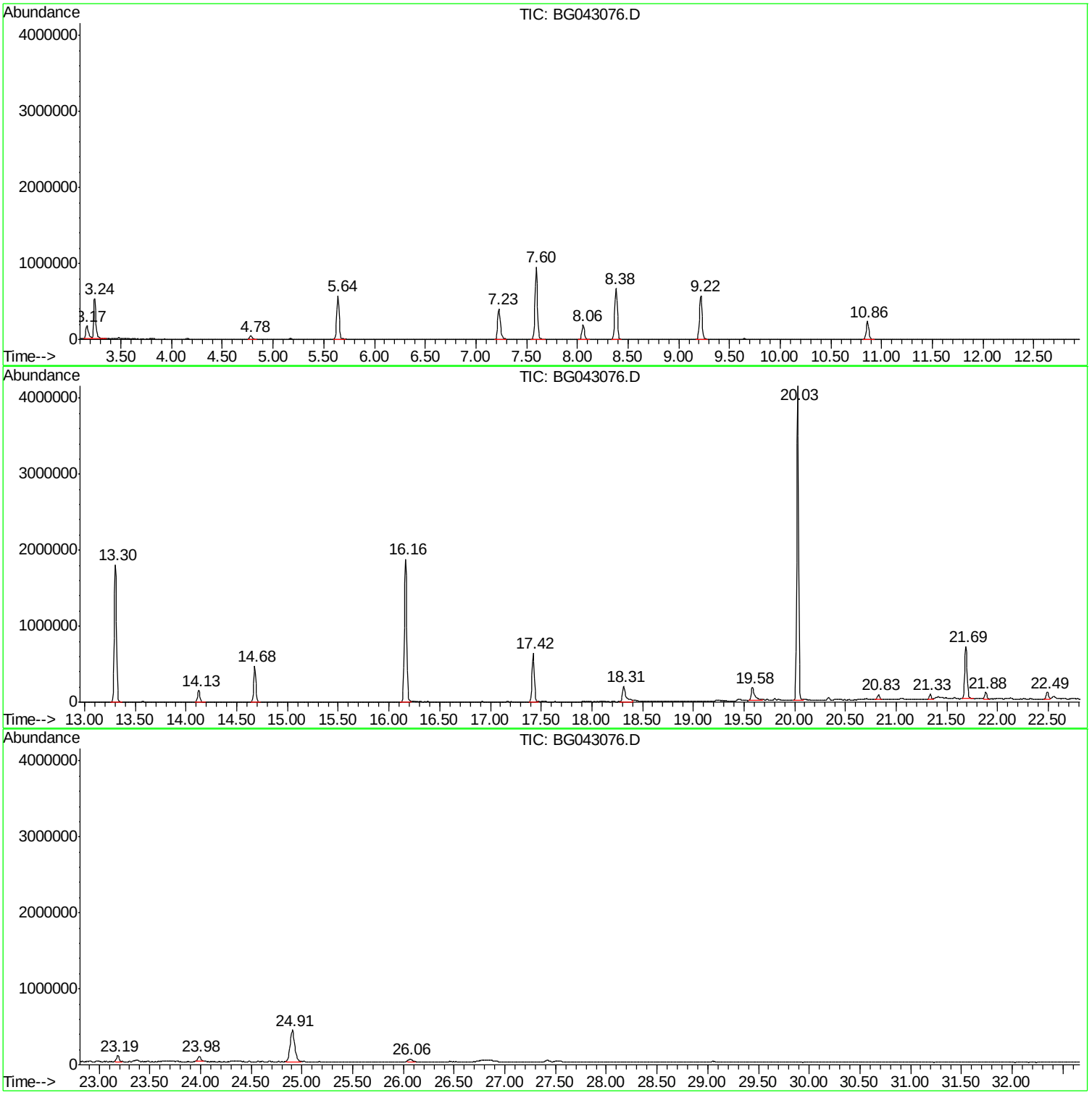
Sum of corrected areas: 25210744

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG100719\
Data File : BG043076.D
Acq On : 7 Oct 2019 20:27
Operator : JU
Sample : K5154-24
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-101S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG100719\
Data File : BG043076.D
Acq On : 7 Oct 2019 20:27
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Sample : K5154-24
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-101S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

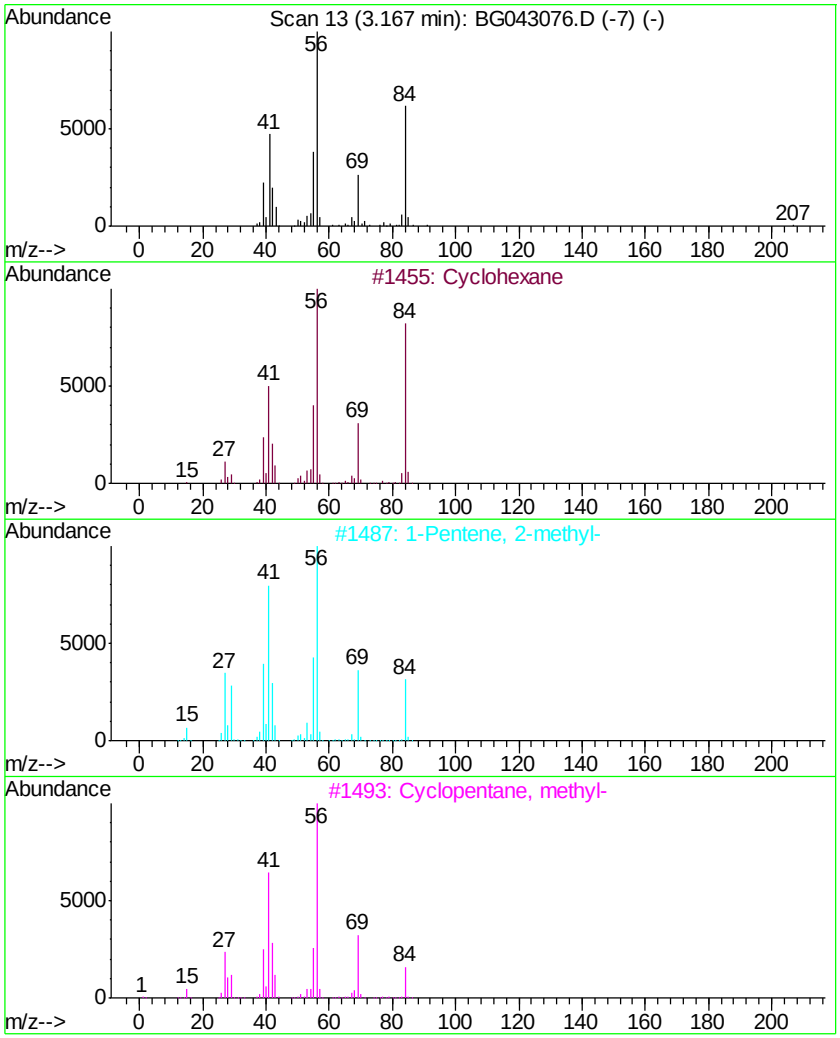
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

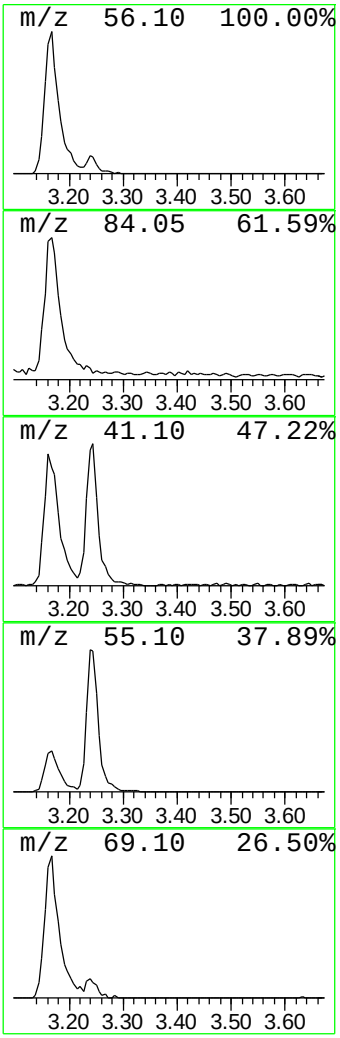
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.17	20.38 ng	331560	1,4-Dichlorobenzene-d4	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane	84	C6H12	000110-82-7	94
2	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	72
3	Cyclopentane, methyl-	84	C6H12	000096-37-7	53
4	2H-Pyran-2,6(3H)-dione, dihydro-...	142	C7H10O3	004160-82-1	50
5	Cyclobutane, ethyl-	84	C6H12	004806-61-5	47





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Data File : BG043076.D
Acq On : 7 Oct 2019 20:27
Operator : JU
Sample : K5154-24
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-101S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

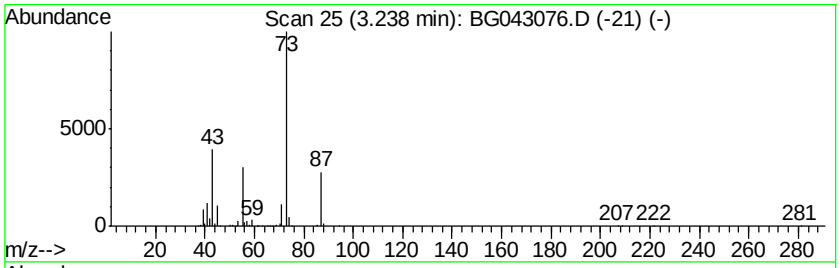
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

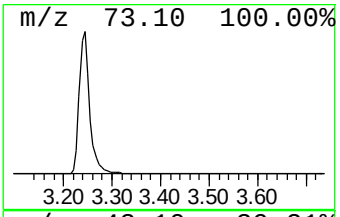
****

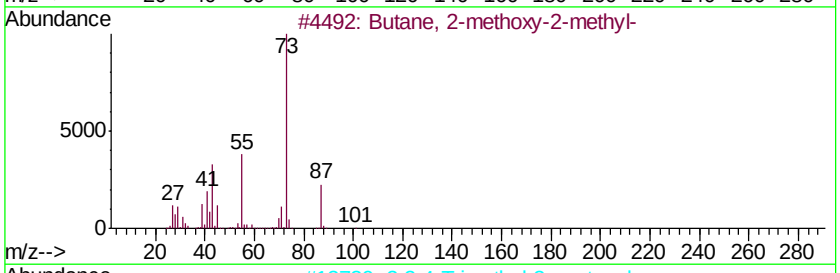
Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 3

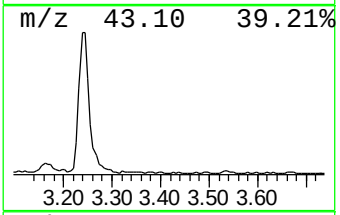
R.T.	EstConc	Area	Relative to ISTD	R.T.
3.24	50.05 ng	814469	1,4-Dichlorobenzene-d4	8.06

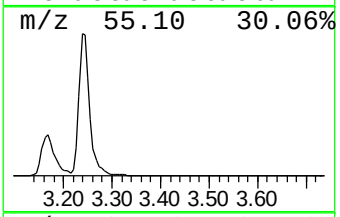
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9

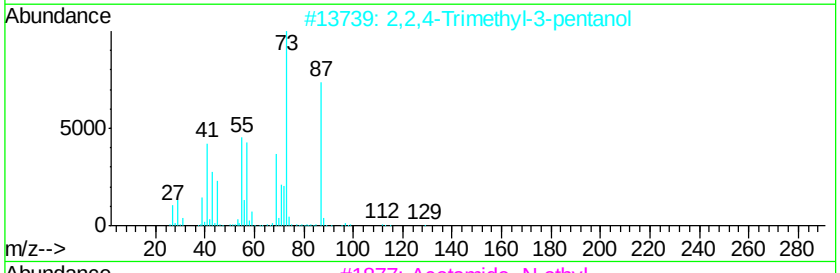


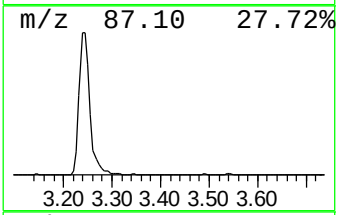


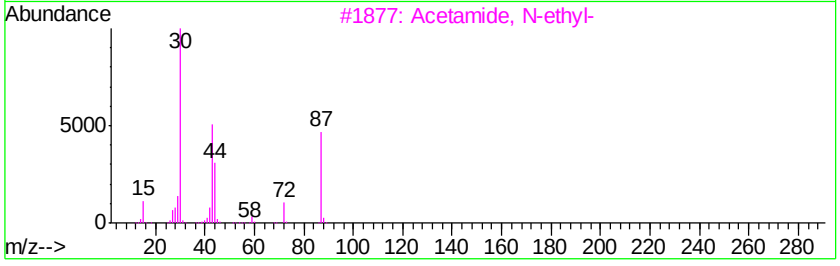


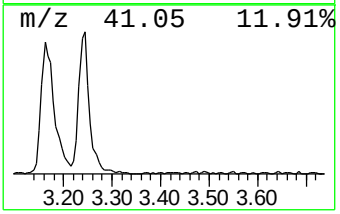












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Acq On : 7 Oct 2019 20:27
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Sample : K5154-24
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-101S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

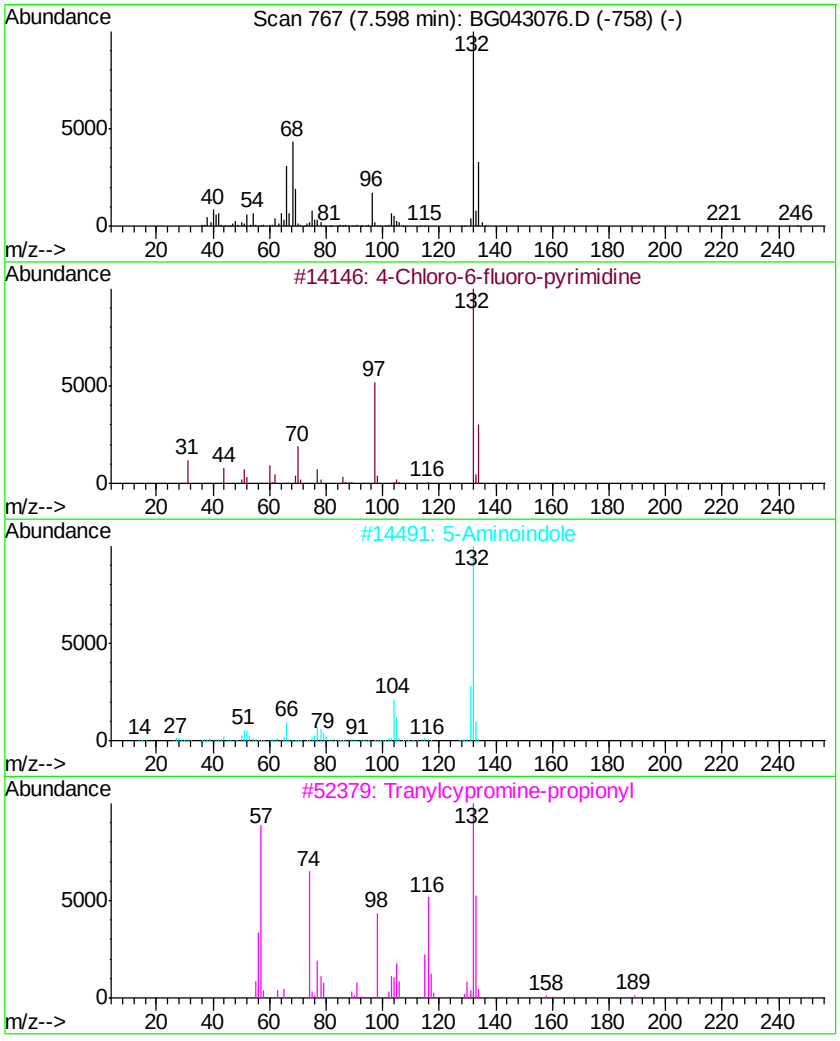
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

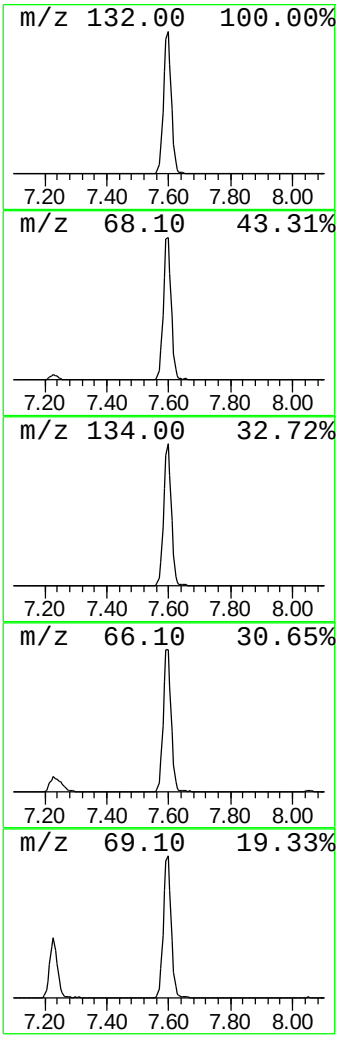
****

Peak Number 4 unknown7.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.60	102.74 ng	1671840	1,4-Dichlorobenzene-d4	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	22
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	10





Library Search Compound Report

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Misc :
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Instrument : BNA_G
ClientSampleId : MW-101S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

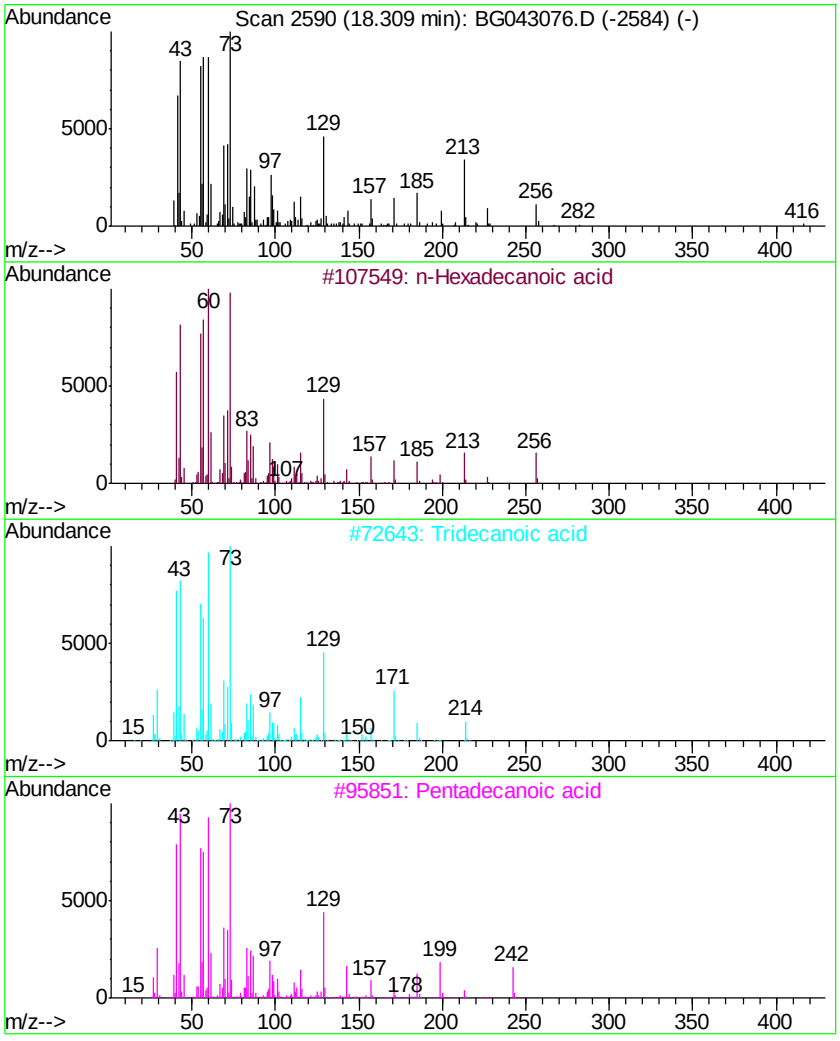
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

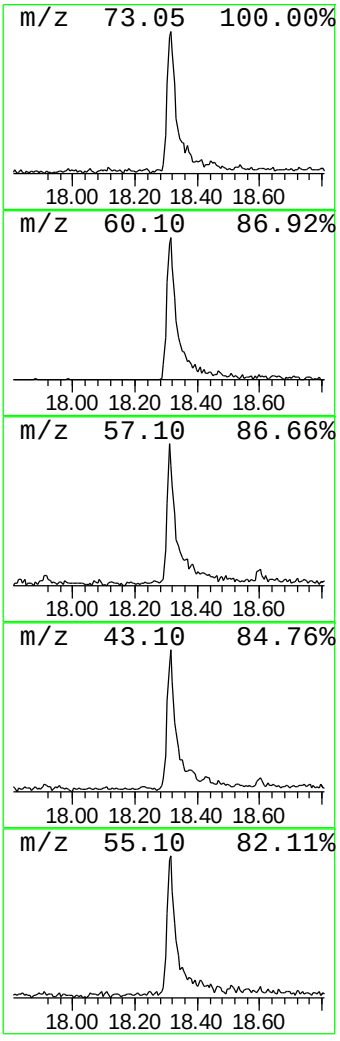
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.31	9.86 ng	485874	Phenanthrene-d10	17.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	n-Decanoic acid	172	C10H20O2	000334-48-5	64
5	Undecanoic acid	186	C11H22O2	000112-37-8	52





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Sample : K5154-24
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-101S

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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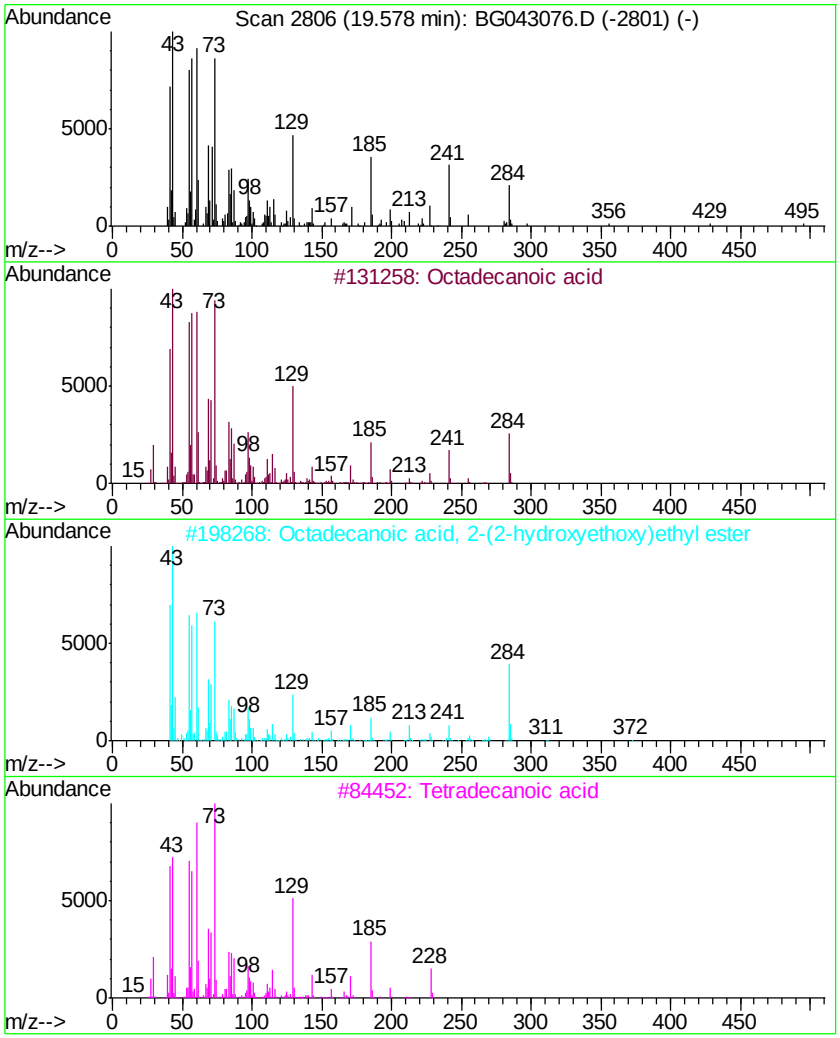
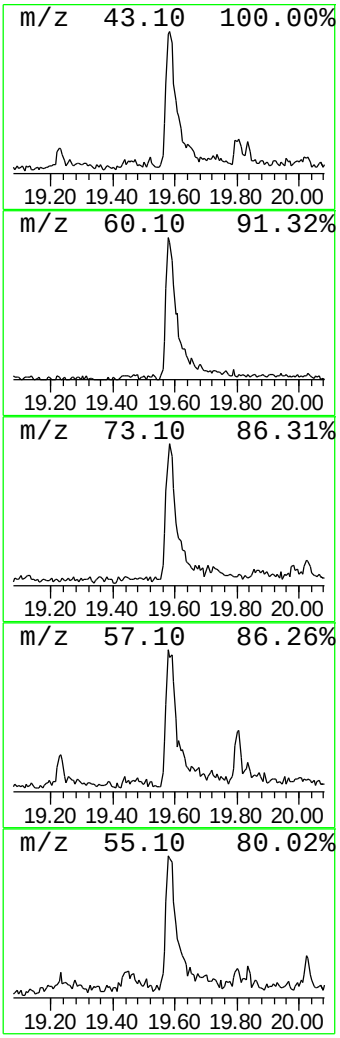
****

Peak Number 7 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.58	7.75 ng	447837	Chrysene-d12	21.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	64





Library Search Compound Report

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Instrument : BNA_G
ClientSampleId : MW-101S

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

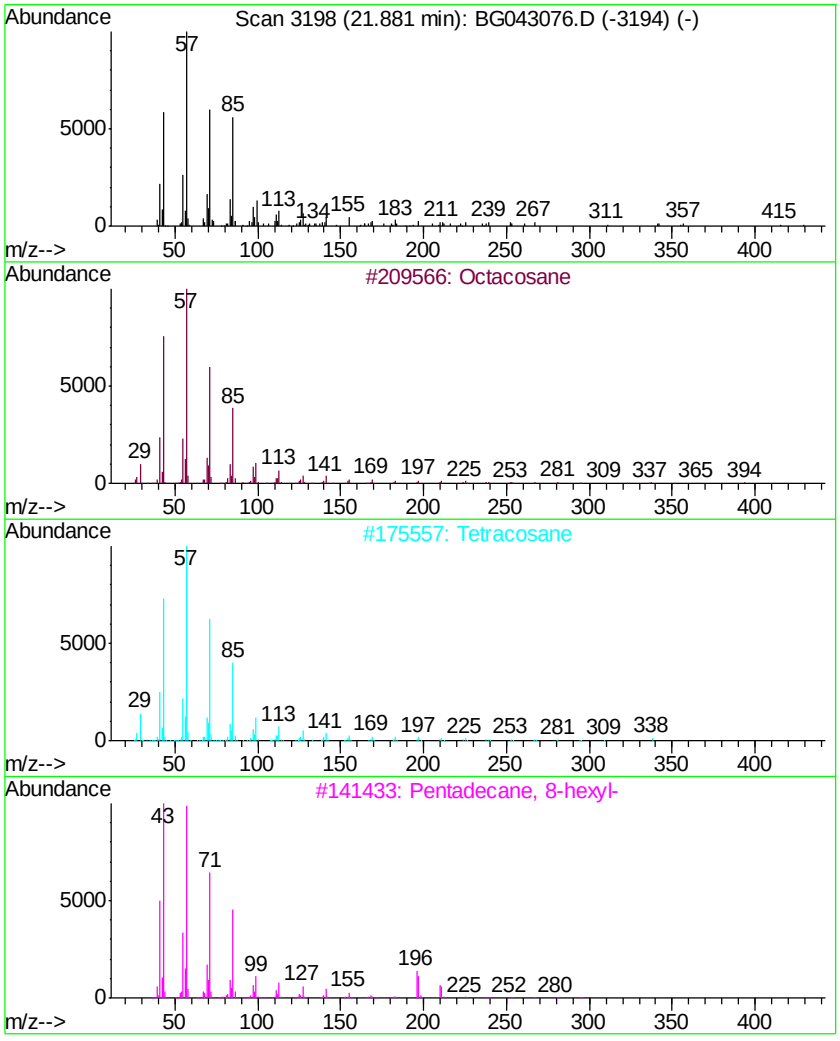
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

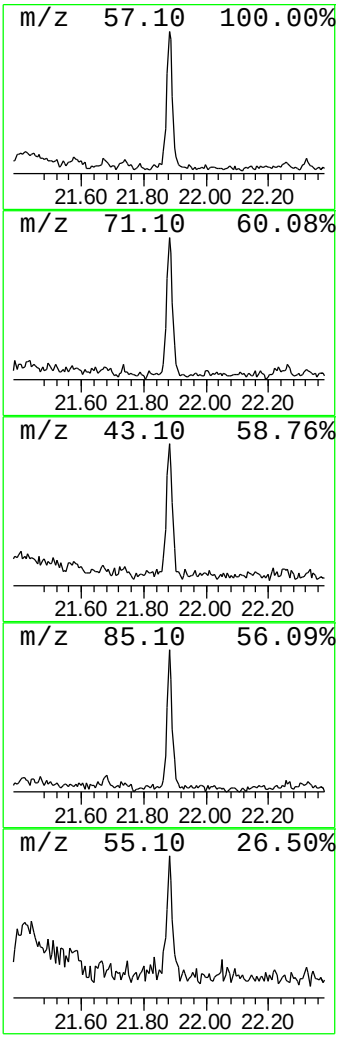
****

Peak Number 8 Octacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.88	2.25 ng	129897	Chrysene-d12	21.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	90
2	Tetracosane	338	C24H50	000646-31-1	87
3	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	86
4	Triacontane	422	C30H62	000638-68-6	76
5	Dodecane, 2-methyl-	184	C13H28	001560-97-0	72





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ClientSampleId : MW-101S

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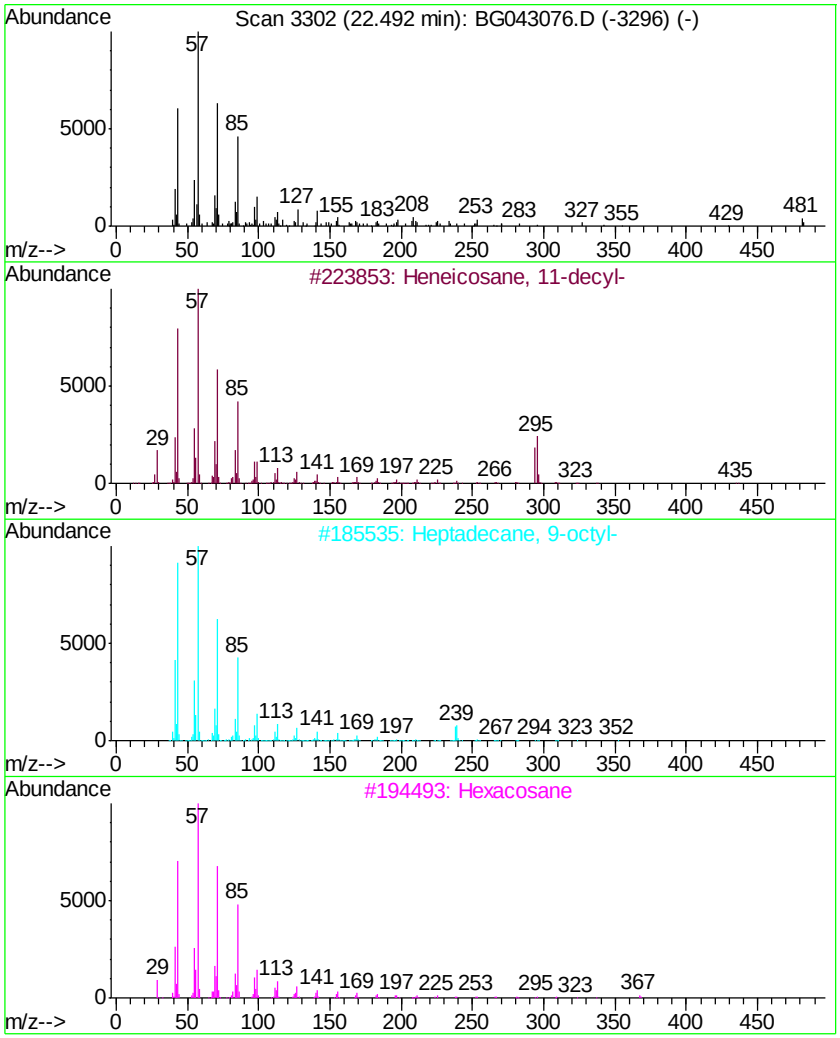
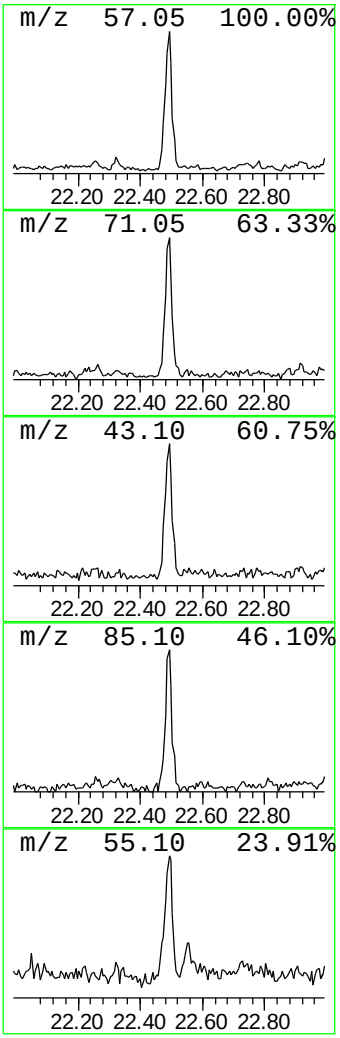
****

Peak Number 9 Heneicosane, 11-decyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.49	2.64 ng	152719	Chrysene-d12	21.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane, 11-decyl-	437	C31H64	055320-06-4	87
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	83
3	Hexacosane	366	C26H54	000630-01-3	83
4	Heptacosane	380	C27H56	000593-49-7	83
5	Tetracosane	338	C24H50	000646-31-1	83





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Misc :
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Instrument : BNA_G
ClientSampleId : MW-101S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

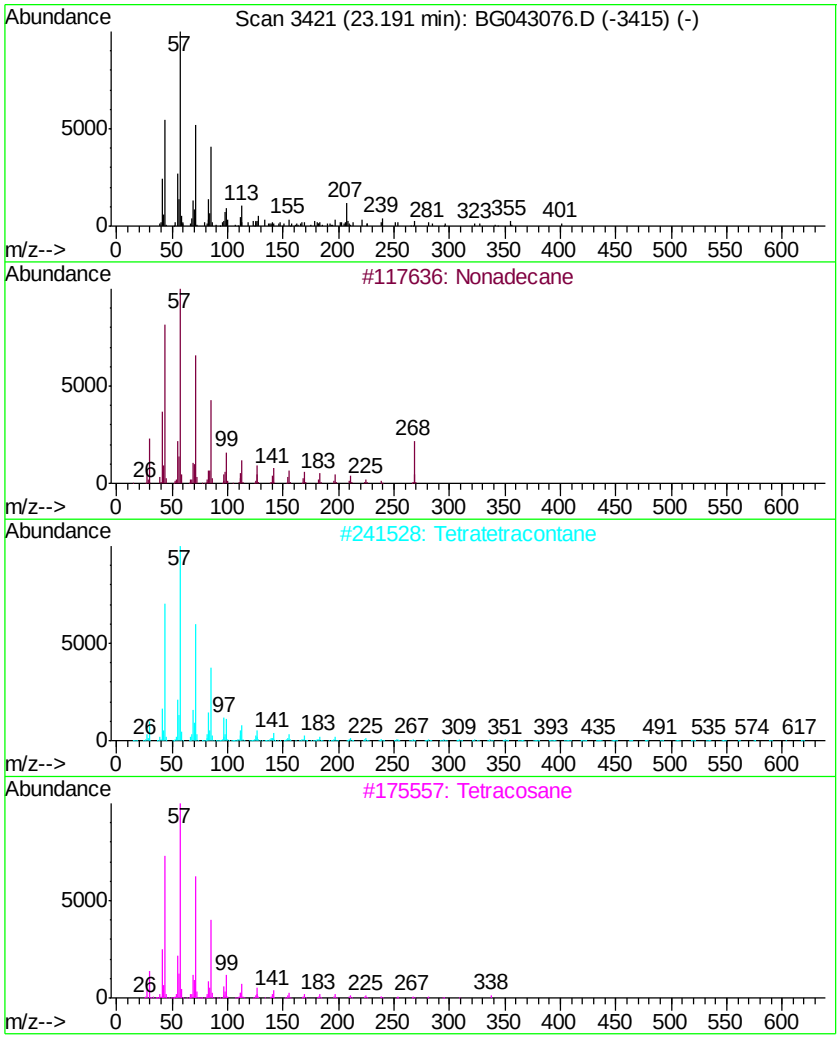
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

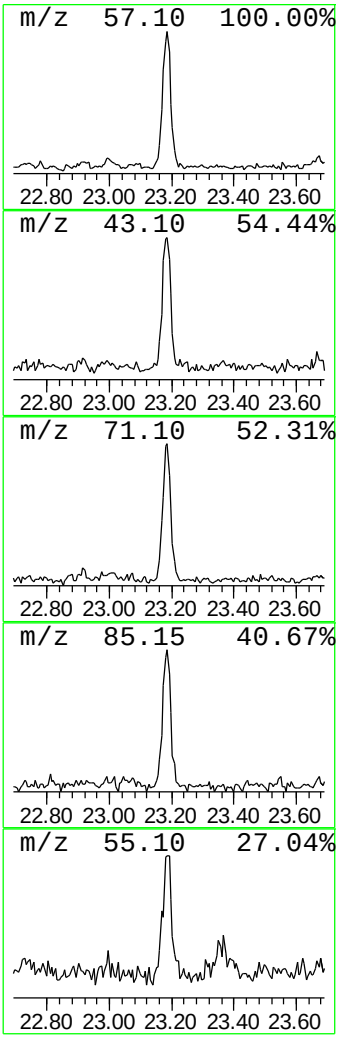
****

Peak Number 10 Nonadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.19	2.41 ng	139254	Chrysene-d12	21.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	91
2	Tetratetracontane	619	C44H90	007098-22-8	90
3	Tetracosane	338	C24H50	000646-31-1	87
4	Hentriacontane	437	C31H64	000630-04-6	87
5	Heptacosane	380	C27H56	000593-49-7	86





Tentatively Identified Compound (LSC) summary

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ClientSampleId : MW-101S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.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
1-Pentene, 2-methyl-	3.17	20.4	ng	331560	1	8.06	325448	20.0
Butane, 2-methoxy...	3.24	50.0	ng	814469	1	8.06	325448	20.0
unknown7.60	7.60	102.7	ng	1671840	1	8.06	325448	20.0
n-Hexadecanoic acid	18.31	9.9	ng	485874	4	17.42	985585	20.0
Octadecanoic acid	19.58	7.8	ng	447837	5	21.69	1155050	20.0
Octacosane	21.88	2.3	ng	129897	5	21.69	1155050	20.0
Heneicosane, 11-d...	22.49	2.6	ng	152719	5	21.69	1155050	20.0
Nonadecane	23.19	2.4	ng	139254	5	21.69	1155050	20.0