LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM050319\
Data File : BM020112.D
Acq On : 03 May 2019 15:16
Operator : JU/SJ
Sample : K2668-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-2

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_M\METHODS\8270-BM043019.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	3.016	3	5	8	rVB	96794	87895	1.22%	0.188%
2	5.363	397	404	415	rVB	2796986	3904652	54.22%	8.334%
3	6.945	665	673	684	rBV	2743966	4215713	58.54%	8.998%
4	7.316	727	736	747	rBV	2891610	4377075	60.78%	9.342%
5	7.787	809	816	822	rBV	506896	765878	10.63%	1.635%
6	8.104	863	870	878	rBV	2018315	3187978	44.27%	6.804%
7	8.951	1006	1014	1024	rBV	1647579	2624112	36.44%	5.601%
8	10.580	1284	1291	1300	rVB	573906	965826	13.41%	2.061%
9	13.045	1703	1710	1717	rVB	3581701	5202421	72.24%	11.104%
10	13.233	1732	1742	1750	rBV2	85557	135025	1.87%	0.288%
11	13.886	1847	1853	1859	rBV	377932	541854	7.52%	1.157%
12	14.316	1920	1926	1933	rBV	132609	185754	2.58%	0.396%
13	14.427	1939	1945	1952	rVB2	857519	1274154	17.69%	2.719%
14	15.268	2082	2088	2092	rVB	157296	192441	2.67%	0.411%
15	15.674	2149	2157	2161	rBV3	42504	78675	1.09%	0.168%
16	15.915	2188	2198	2208	rBV	3304542	4680728	64.99%	9.990%
17	16.127	2229	2234	2242	rBV	169662	301715	4.19%	0.644%
18	16.921	2364	2369	2373	rBV	132173	158088	2.20%	0.337%
19	17.174	2405	2412	2417	rBV	1151809	1596933	22.17%	3.408%
20	17.656	2490	2494	2502	rVB	112793	139194	1.93%	0.297%
21	18.056	2557	2562	2568	rBV	160534	250848	3.48%	0.535%
22	18.351	2608	2612	2618	rBV	93891	108285	1.50%	0.231%
23	19.339	2775	2780	2784	rBV3	77014	120790	1.68%	0.258%
24	19.797	2853	2858	2864	rVB	5997532	7201805	100.00%	15.371%
25	21.056	3069	3072	3077	rVB2	139729	154284	2.14%	0.329%
26	21.356	3118	3123	3128	rBV	1387506	1729511	24.01%	3.691%
27	21.497	3144	3147	3152	rVB2	65824	77111	1.07%	0.165%
28	21.939	3219	3222	3228	rBV5	87129	151287	2.10%	0.323%
29	22.409	3299	3302	3306	rVB	96565	115010	1.60%	0.245%
30	22.927	3386	3390	3395	rVB	175124	241333	3.35%	0.515%
31	23.509	3486	3489	3494	rVB3	96013	143325	1.99%	0.306%
32	23.638	3505	3511	3520	rVB	887161	1750075	24.30%	3.735%
33	24.174	3599	3602	3610	rVB3	98750	192916	2.68%	0.412%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM050319\
Data File : BM020112.D
Acq On : 03 May 2019 15:16
Operator : JU/SJ
Sample : K2668-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-2

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_M\METHODS\8270-BM043019.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

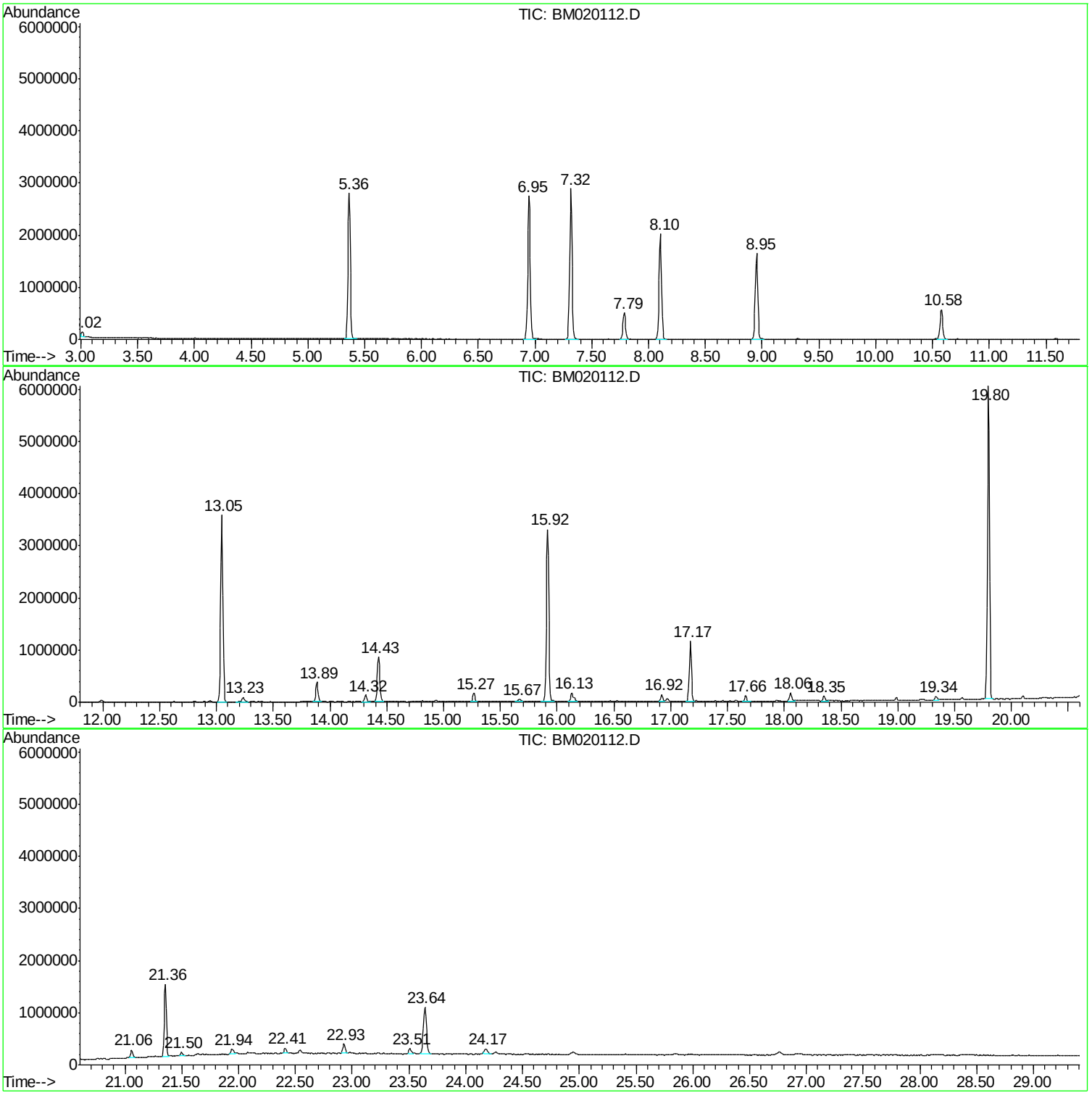
Sum of corrected areas: 46852691

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM050319\
Data File : BM020112.D
Acq On : 03 May 2019 15:16
Operator : JU/SJ
Sample : K2668-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM043019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM050319\
Data File : BM020112.D
Acq On : 03 May 2019 15:16
Operator : JU/SJ
Sample : K2668-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM043019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

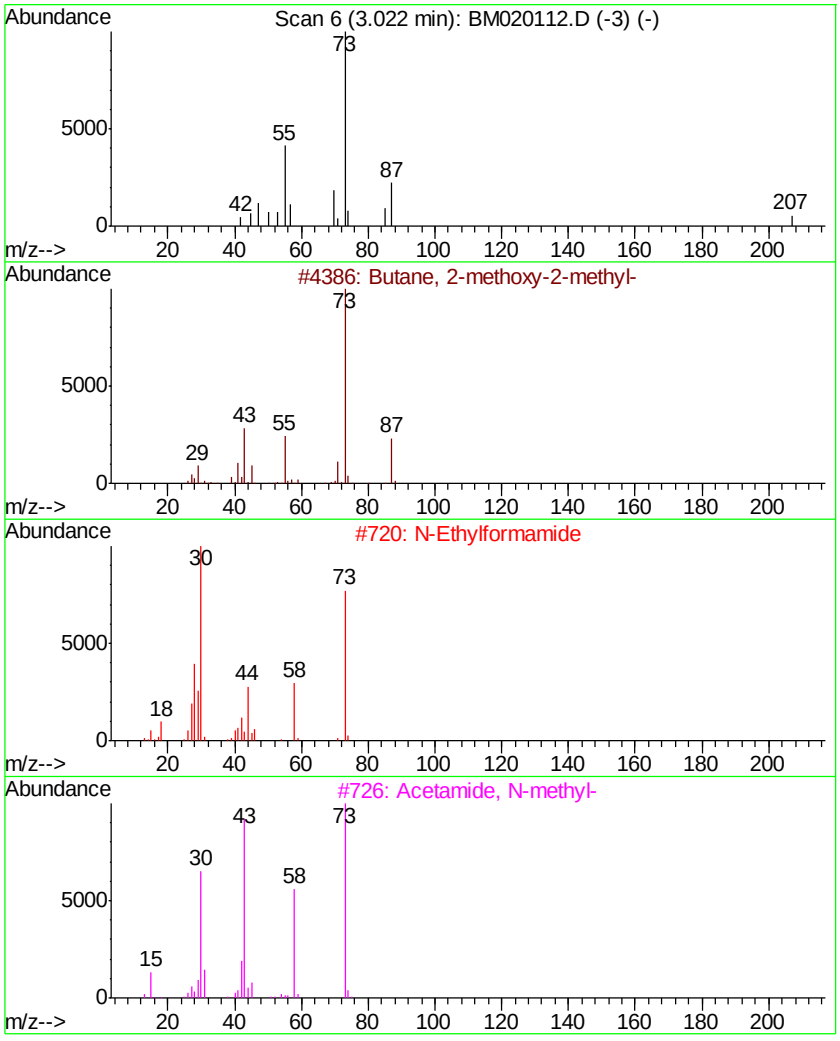
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

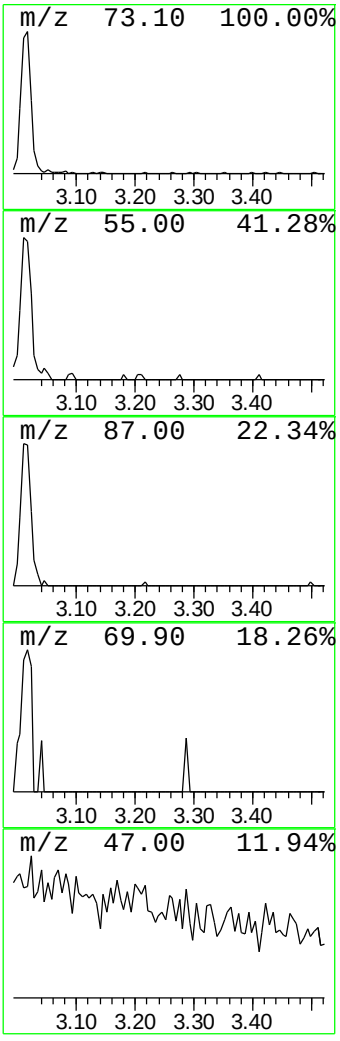
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.02	2.30 ng	87895	1,4-Dichlorobenzene-d4	7.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	N-Ethylformamide	73	C3H7NO	000627-45-2	17
3	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	2-(2-Bromoethyl)-1,3-dioxolane	180	C5H9BrO2	018742-02-4	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM050319\
Data File : BM020112.D
Acq On : 03 May 2019 15:16
Operator : JU/SJ
Sample : K2668-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM043019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

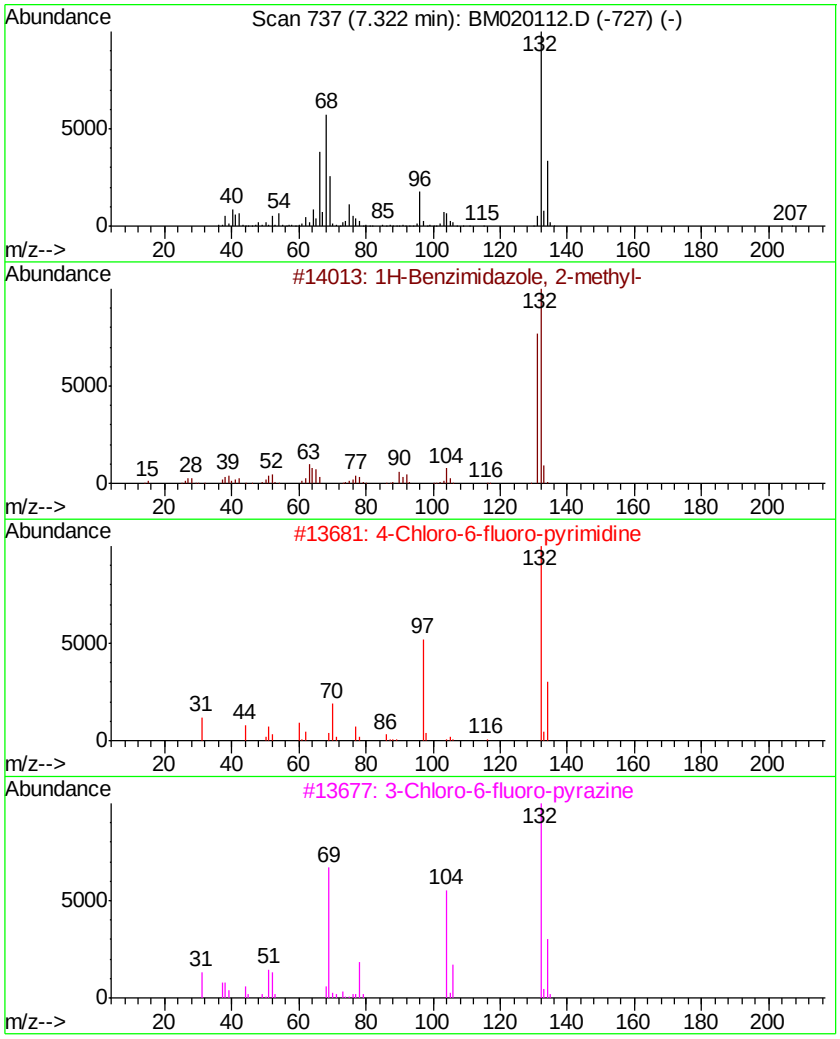
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

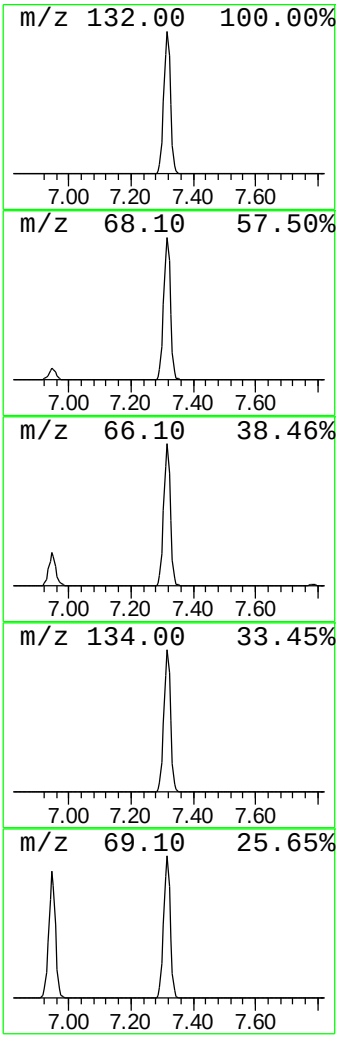
****

Peak Number 2 unknown7.32 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.32	114.30 ng	4377080	1,4-Dichlorobenzene-d4	7.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
3	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	10
5	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	10





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM050319\
Data File : BM020112.D
Acq On : 03 May 2019 15:16
Operator : JU/SJ
Sample : K2668-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM043019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

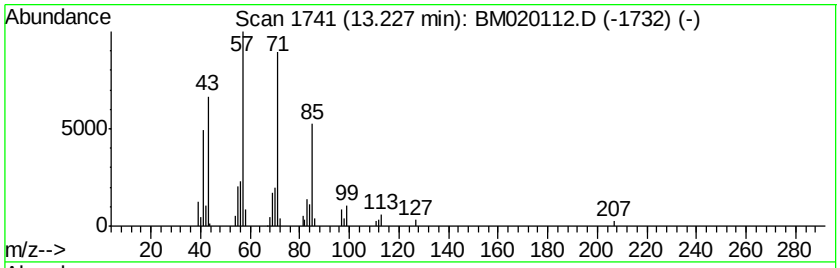
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

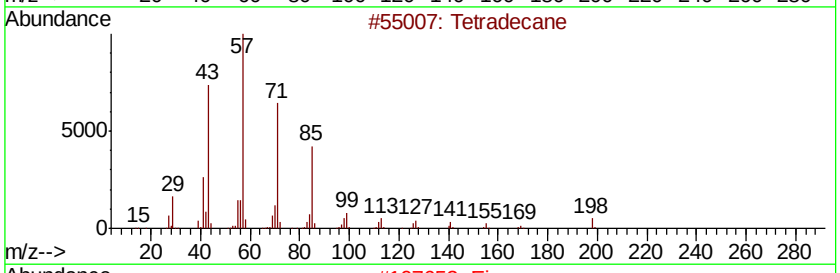
****

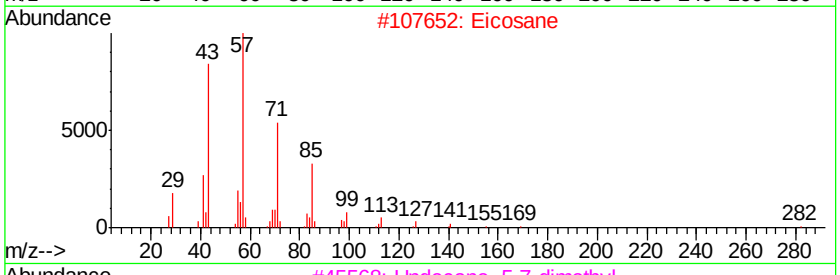
Peak Number 4 Tetradecane Concentration Rank 10

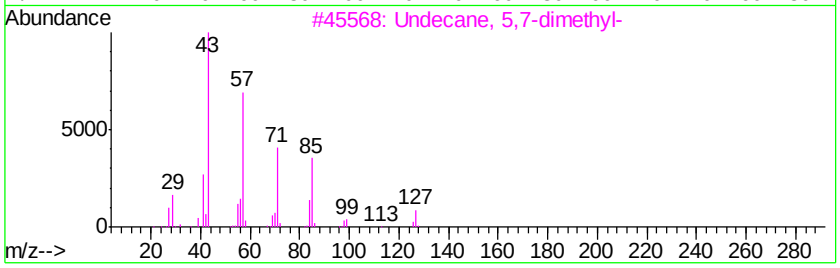
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.23	2.12 ng	135025	Acenaphthene-d10	14.43

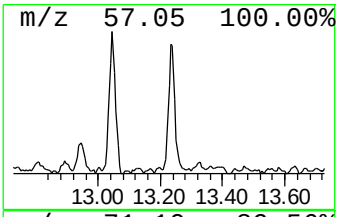
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	91
2	Eicosane	282	C20H42	000112-95-8	80
3	Undecane, 5,7-dimethyl-	184	C13H28	017312-83-3	80
4	Undecane, 2,3-dimethyl-	184	C13H28	017312-77-5	78
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	78

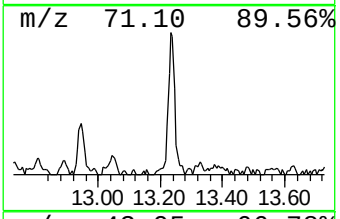


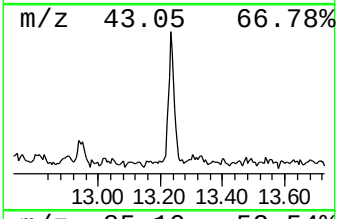


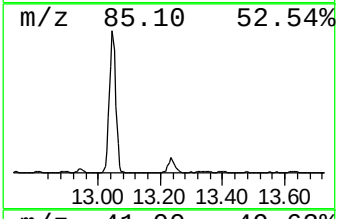


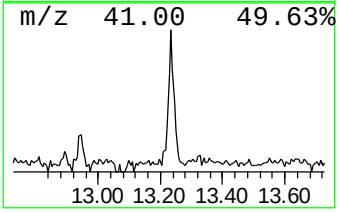












Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM050319\
Data File : BM020112.D
Acq On : 03 May 2019 15:16
Operator : JU/SJ
Sample : K2668-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM043019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

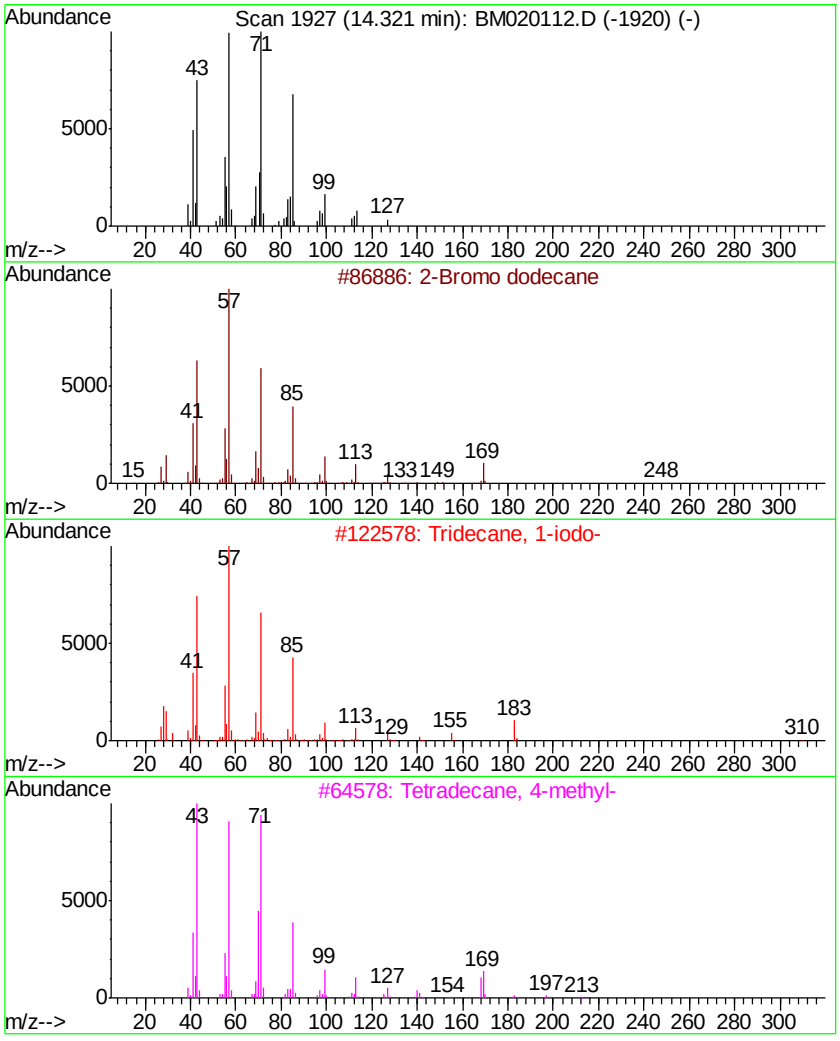
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

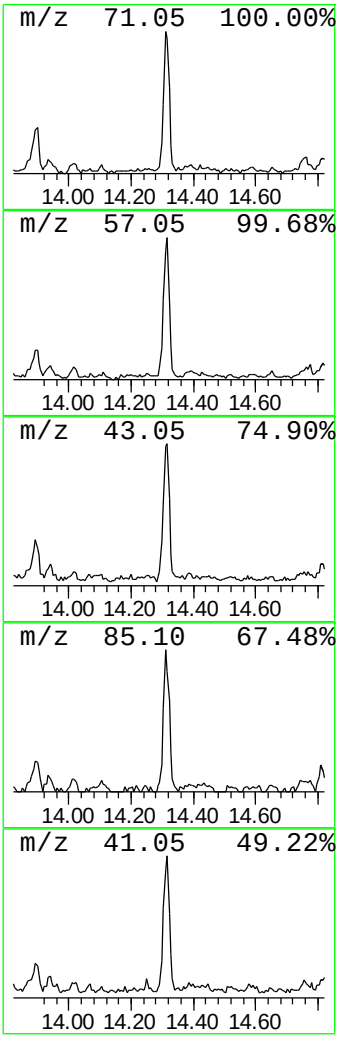
****

Peak Number 5 2-Bromo dodecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.32	2.92 ng	185754	Acenaphthene-d10	14.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromo dodecane	248	C12H25Br	013187-99-0	90
2	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	90
3	Tetradecane, 4-methyl-	212	C15H32	025117-24-2	86
4	Heptacosane	380	C27H56	000593-49-7	72
5	Eicosane	282	C20H42	000112-95-8	64





Library Search Compound Report

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Data File : BM020112.D
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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM043019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

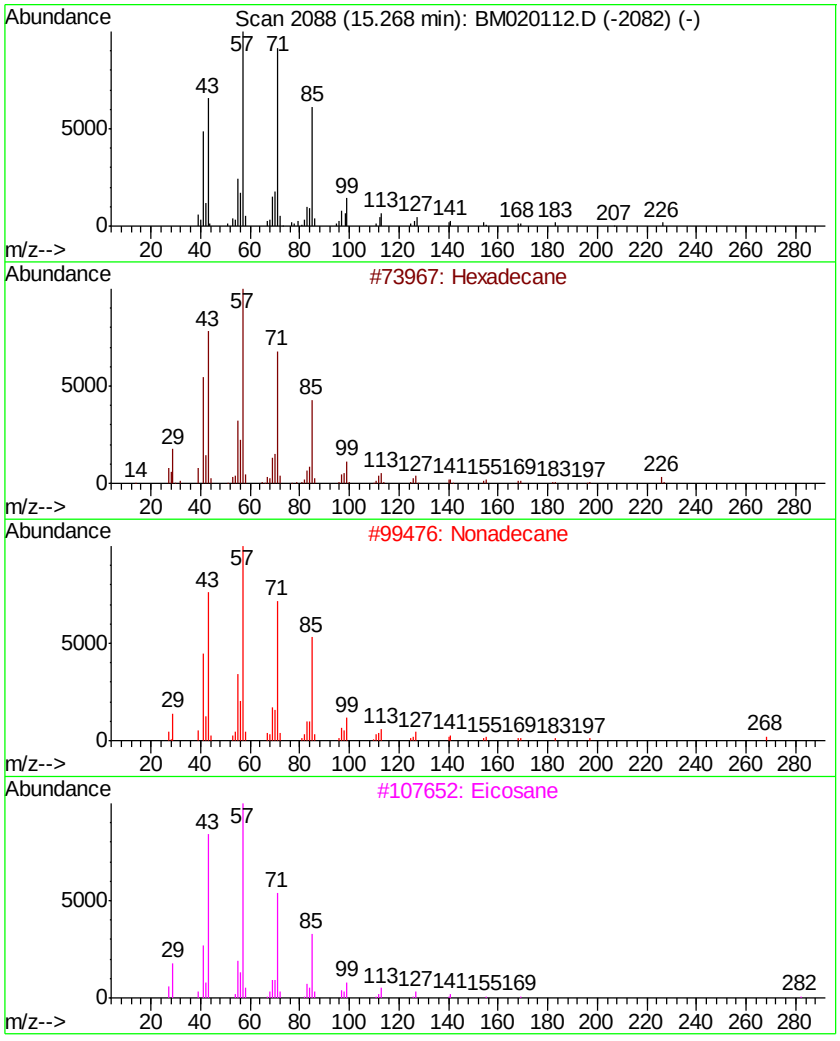
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

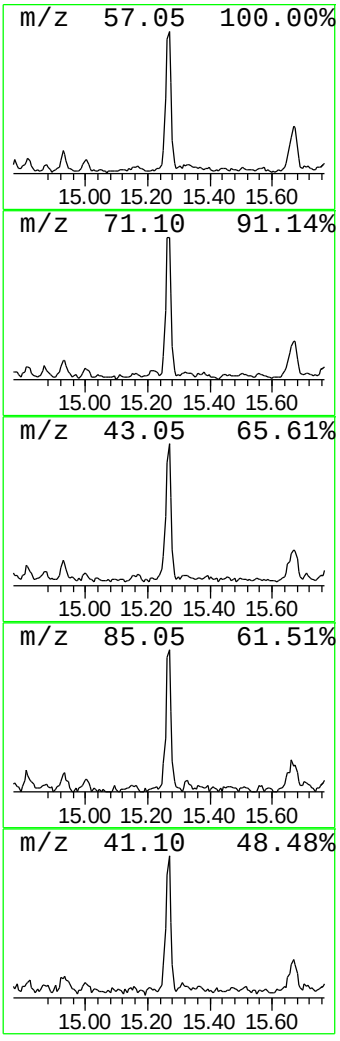
****

Peak Number 6 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.27	3.02 ng	192441	Acenaphthene-d10	14.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	95
2	Nonadecane	268	C19H40	000629-92-5	91
3	Eicosane	282	C20H42	000112-95-8	87
4	Pentadecane	212	C15H32	000629-62-9	80
5	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	72





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM050319\
Data File : BM020112.D
Acq On : 03 May 2019 15:16
Operator : JU/SJ
Sample : K2668-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM043019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

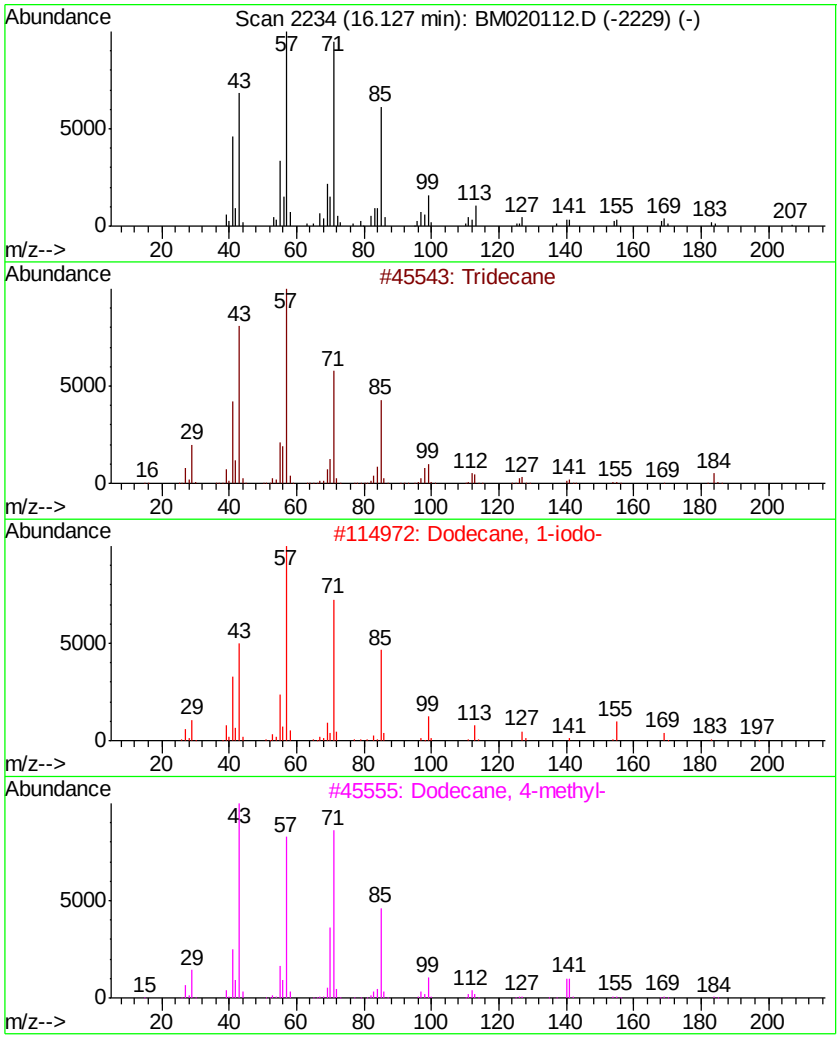
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

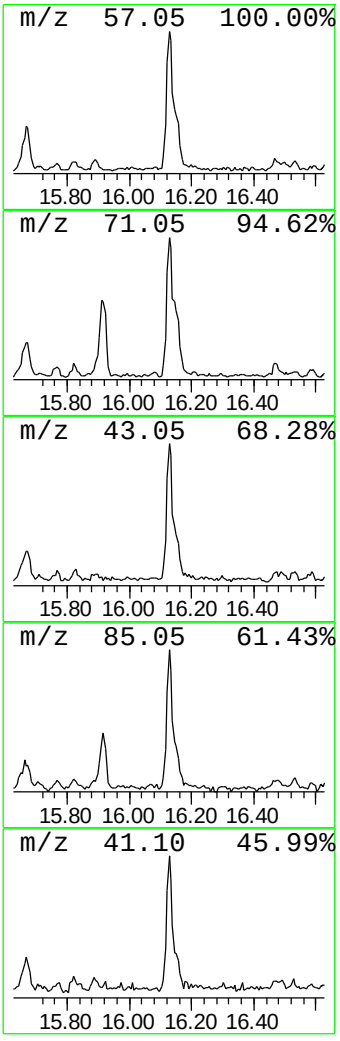
****

Peak Number 7 Tridecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	3.78 ng	301715	Phenanthrene-d10	17.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	87
2	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
3	Dodecane, 4-methyl-	184	C13H28	006117-97-1	86
4	Undecane, 6-ethyl-	184	C13H28	017312-60-6	81
5	Undecane, 2,3-dimethyl-	184	C13H28	017312-77-5	80





Library Search Compound Report

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Acq On : 03 May 2019 15:16
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ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM043019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

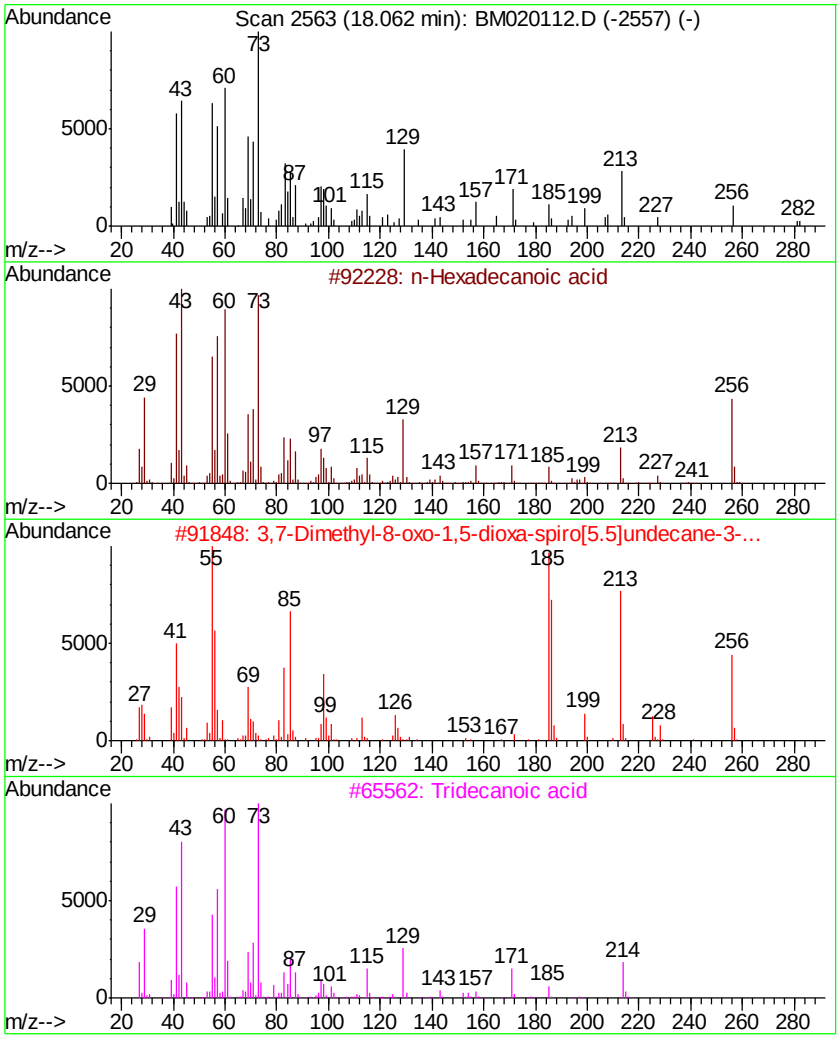
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

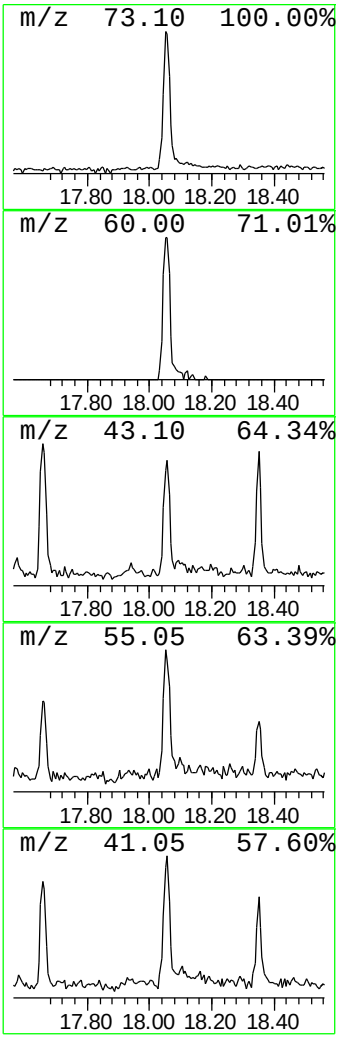
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.06	3.14 ng	250848	Phenanthrene-d10	17.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	3,7-Dimethyl-8-oxo-1,5-dioxa-spi...	256	C13H20O5	1000193-79-8	35
3	Tridecanoic acid	214	C13H26O2	000638-53-9	22
4	Octadecane, 2-methyl-	268	C19H40	001560-88-9	18
5	Nonanoic acid	158	C9H18O2	000112-05-0	18





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM050319\
Data File : BM020112.D
Acq On : 03 May 2019 15:16
Operator : JU/SJ
Sample : K2668-03
Misc :
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Instrument : BNA_M
ClientSampleId : TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM043019.M
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TIC Library : C:\DATABASE\NIST02.L
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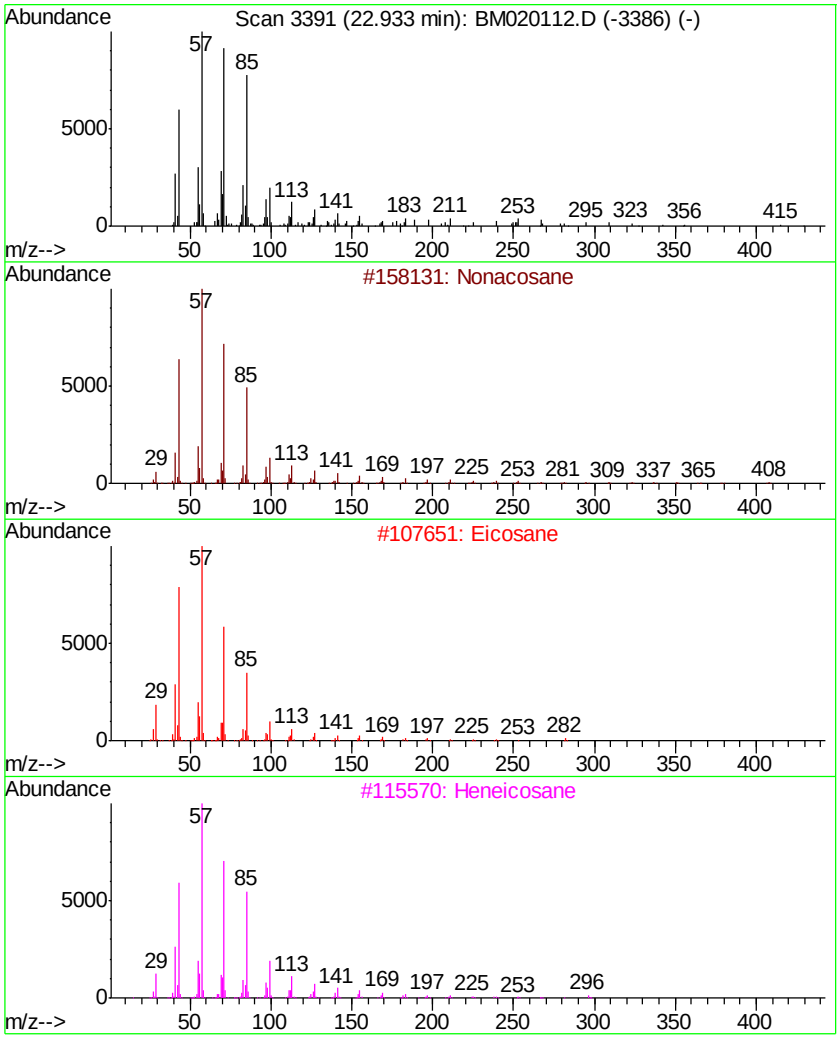
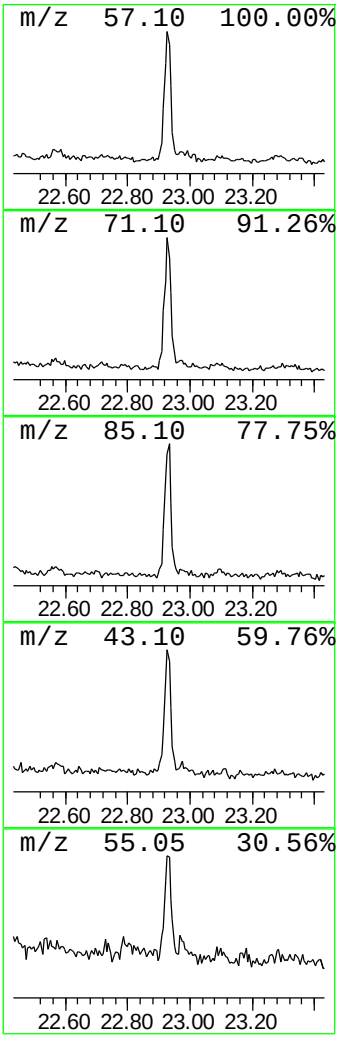
****

Peak Number 9 Nonacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.93	2.76 ng	241333	Perylene-d12	23.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonacosane	408	C29H60	000630-03-5	87
2	Eicosane	282	C20H42	000112-95-8	86
3	Heneicosane	296	C21H44	000629-94-7	83
4	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	80
5	Heptacosane	380	C27H56	000593-49-7	72





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM050319\
Data File : BM020112.D
Acq On : 03 May 2019 15:16
Operator : JU/SJ
Sample : K2668-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM043019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

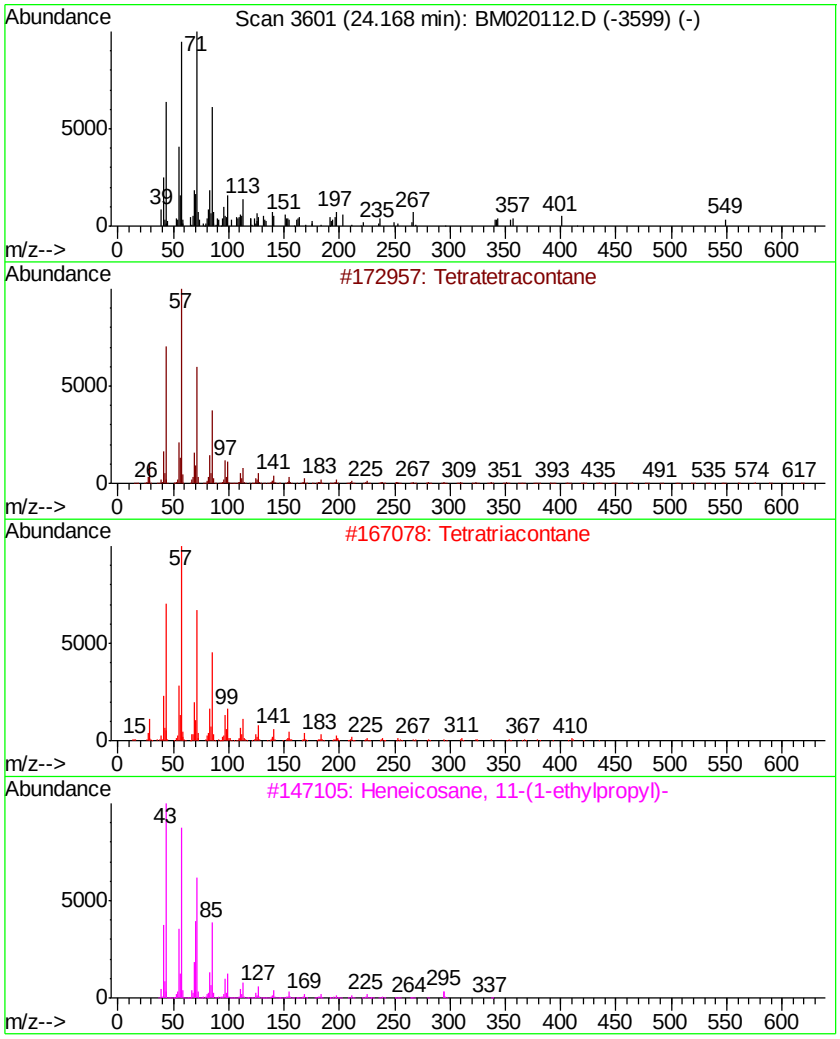
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

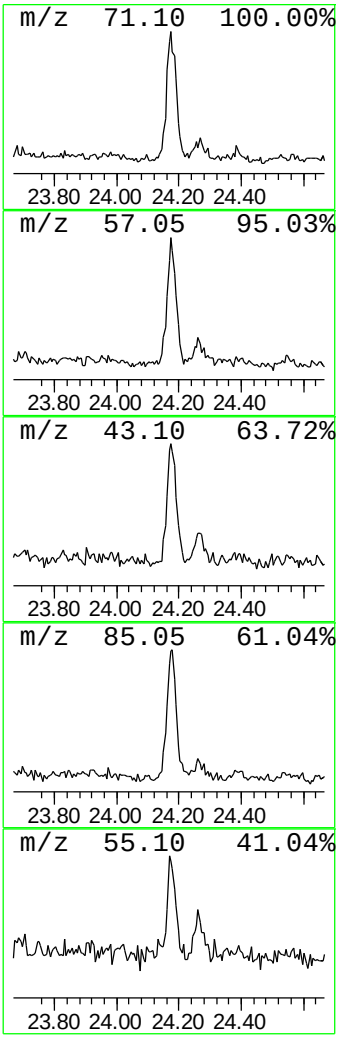
****

Peak Number 10 Tetratetracontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.17	2.20 ng	192916	Perylene-d12	23.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	87
2	Tetratriacontane	479	C34H70	014167-59-0	83
3	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	80
4	Hentriacontane	437	C31H64	000630-04-6	80
5	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM050319\
Data File : BM020112.D
Acq On : 03 May 2019 15:16
Operator : JU/SJ
Sample : K2668-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM043019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	3.02	2.3	ng	87895	1	7.79	765878	20.0
unknown7.32	7.32	114.3	ng	4377080	1	7.79	765878	20.0
Tetradecane	13.23	2.1	ng	135025	3	14.43	1274150	20.0
2-Bromo dodecane	14.32	2.9	ng	185754	3	14.43	1274150	20.0
Hexadecane	15.27	3.0	ng	192441	3	14.43	1274150	20.0
Tridecane	16.13	3.8	ng	301715	4	17.17	1596930	20.0
n-Hexadecanoic acid	18.06	3.1	ng	250848	4	17.17	1596930	20.0
Nonacosane	22.93	2.8	ng	241333	6	23.64	1750080	20.0
Tetratetracontane	24.17	2.2	ng	192916	6	23.64	1750080	20.0