LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121918\
Data File : BM018299.D
Acq On : 19 Dec 2018 15:44
Operator : JU/SJ
Sample : J6446-20
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P001-SS023-1218-01

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-BM121518.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	4.675	300	304	312	rBV	82296	120292	2.31%	0.343%
2	5.122	374	380	391	rBV	2022197	2879468	55.24%	8.208%
3	6.687	639	646	659	rBV	1864656	3215175	61.68%	9.165%
4	7.028	697	704	714	rBV	2105665	3236214	62.08%	9.225%
5	7.487	776	782	791	rBV	386279	595394	11.42%	1.697%
6	7.798	826	835	844	rBV	1489136	2355093	45.18%	6.714%
7	8.645	972	979	993	rBV	1079929	1857783	35.64%	5.296%
8	10.251	1242	1252	1267	rBV	415018	761686	14.61%	2.171%
9	12.751	1670	1677	1689	rBV	2445470	3695235	70.89%	10.534%
10	13.621	1818	1825	1835	rBV	140843	239463	4.59%	0.683%
11	14.145	1907	1914	1928	rVB2	610641	956195	18.34%	2.726%
12	15.651	2164	2170	2184	rBV	1971839	3054999	58.61%	8.709%
13	16.910	2378	2384	2399	rBV	731863	1113273	21.36%	3.174%
14	17.821	2534	2539	2556	rBV	295400	473141	9.08%	1.349%
15	19.115	2755	2759	2766	rBV3	114035	183297	3.52%	0.523%
16	19.562	2829	2835	2844	rBV	4348920	5212616	100.00%	14.859%
17	19.851	2880	2884	2886	rBV4	32921	54607	1.05%	0.156%
18	20.850	3050	3054	3061	rBV	582735	740717	14.21%	2.112%
19	21.127	3096	3101	3113	rBV	1200043	1564414	30.01%	4.460%
20	21.292	3126	3129	3135	rVB4	71804	85047	1.63%	0.242%
21	21.709	3197	3200	3202	rBV	159783	199825	3.83%	0.570%
22	21.733	3202	3204	3213	rVB2	281821	410890	7.88%	1.171%
23	22.156	3273	3276	3280	rBV2	200935	256406	4.92%	0.731%
24	22.633	3354	3357	3363	rVB	211655	295638	5.67%	0.843%
25	23.286	3462	3468	3475	rBV	827195	1522544	29.21%	4.340%

Sum of corrected areas: 35079412

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121918\
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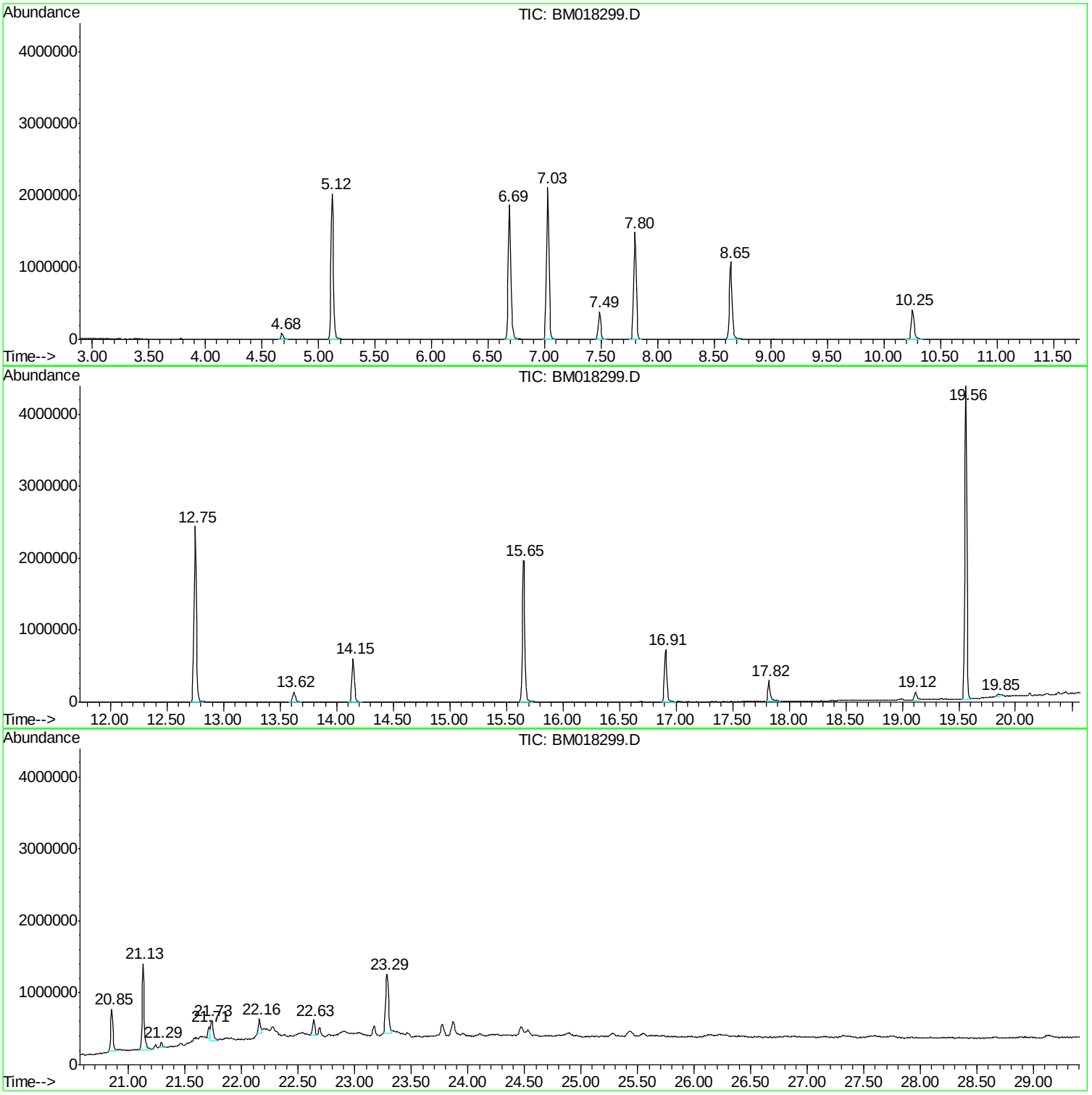
Acq On : 19 Dec 2018 15:44
Operator : JU/SJ
Sample : J6446-20
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P001-SS023-1218-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM121518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BM018299.D
Acq On : 19 Dec 2018 15:44
Operator : JU/SJ
Sample : J6446-20
Misc :
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Instrument : BNA_M
ClientSampleId : P001-SS023-1218-01

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TIC Integration Parameters: LSCINT.P

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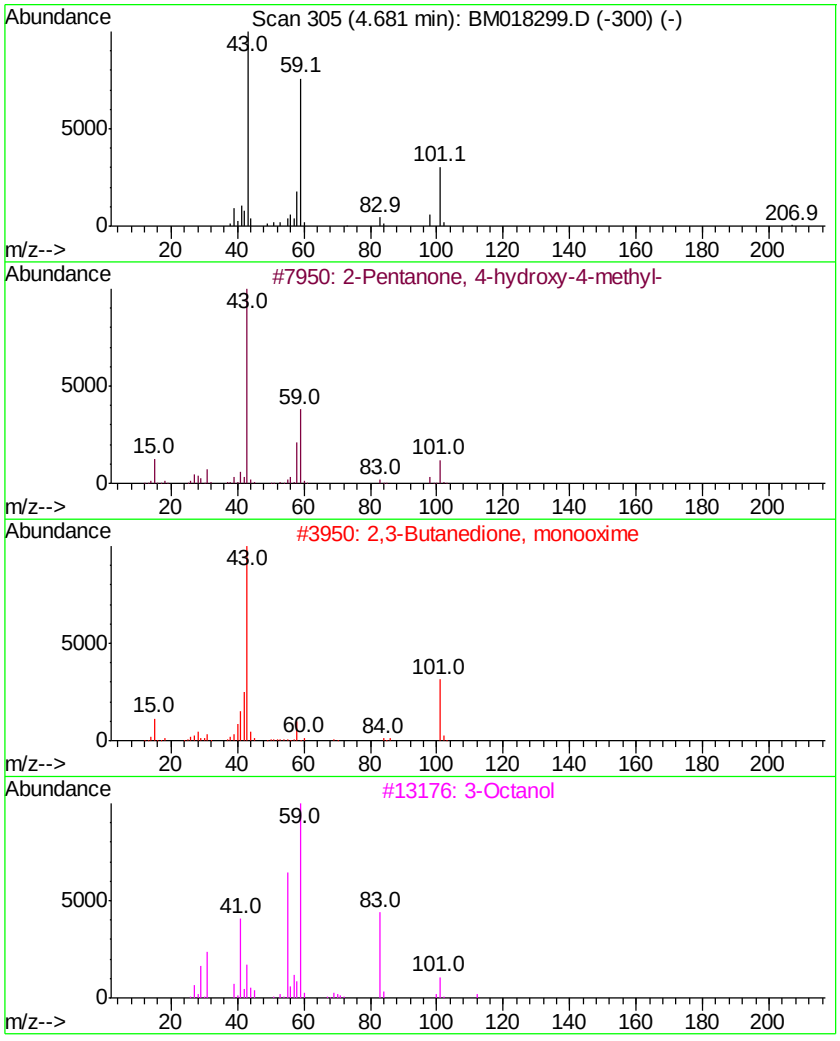
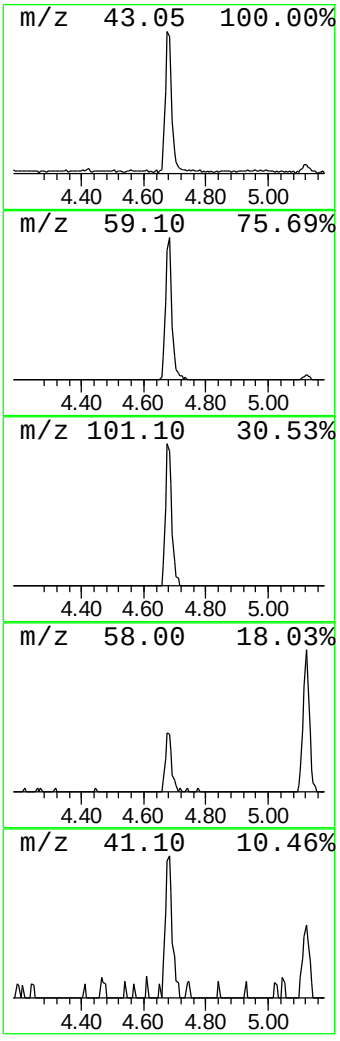
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.68	4.04 ng	120292	1,4-Dichlorobenzene-d4	7.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	32
3	3-Octanol	130	C8H18O	000589-98-0	17
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	12
5	1-Butene, 4-ethoxy-	100	C6H12O	044611-46-3	10





Library Search Compound Report

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Acq On : 19 Dec 2018 15:44
Operator : JU/SJ
Sample : J6446-20
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P001-SS023-1218-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM121518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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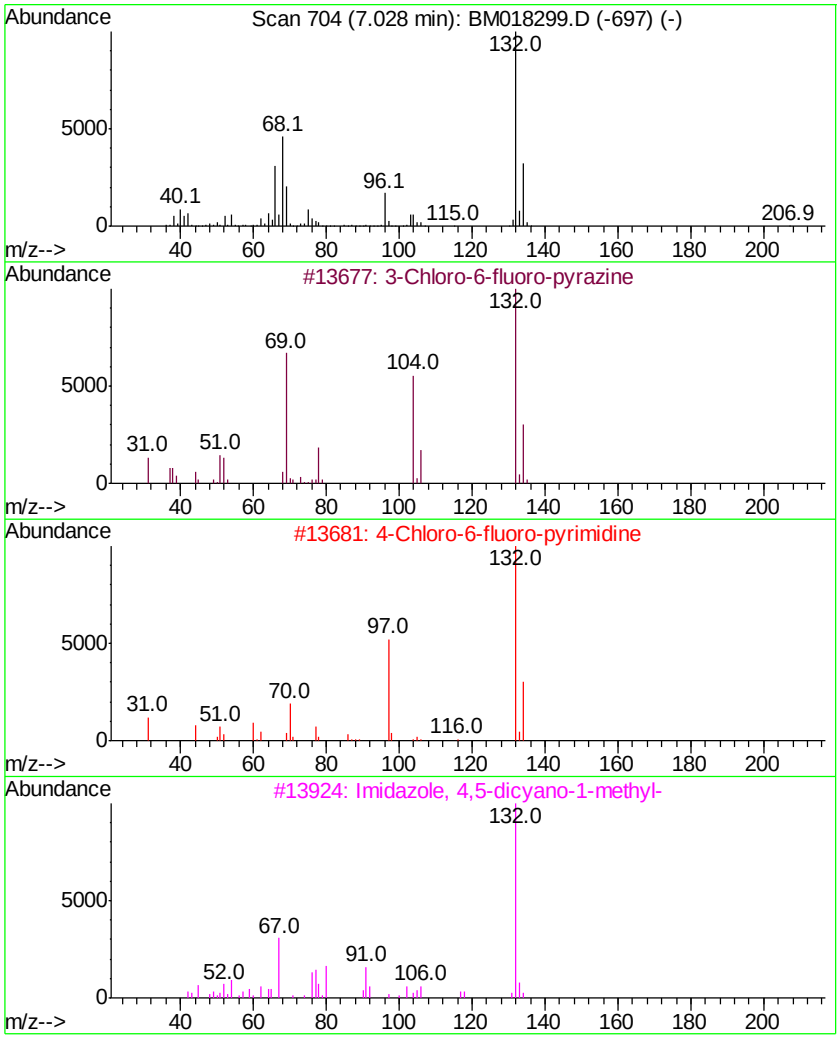
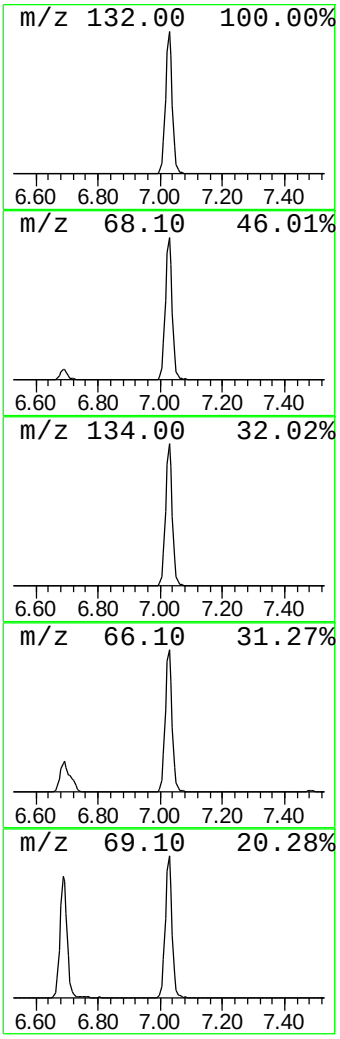
Peak Number 2 unknown7.03 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.03	108.71 ng	3236210	1,4-Dichlorobenzene-d4	7.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	25
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	22





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Operator : JU/SJ
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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P001-SS023-1218-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM121518.M
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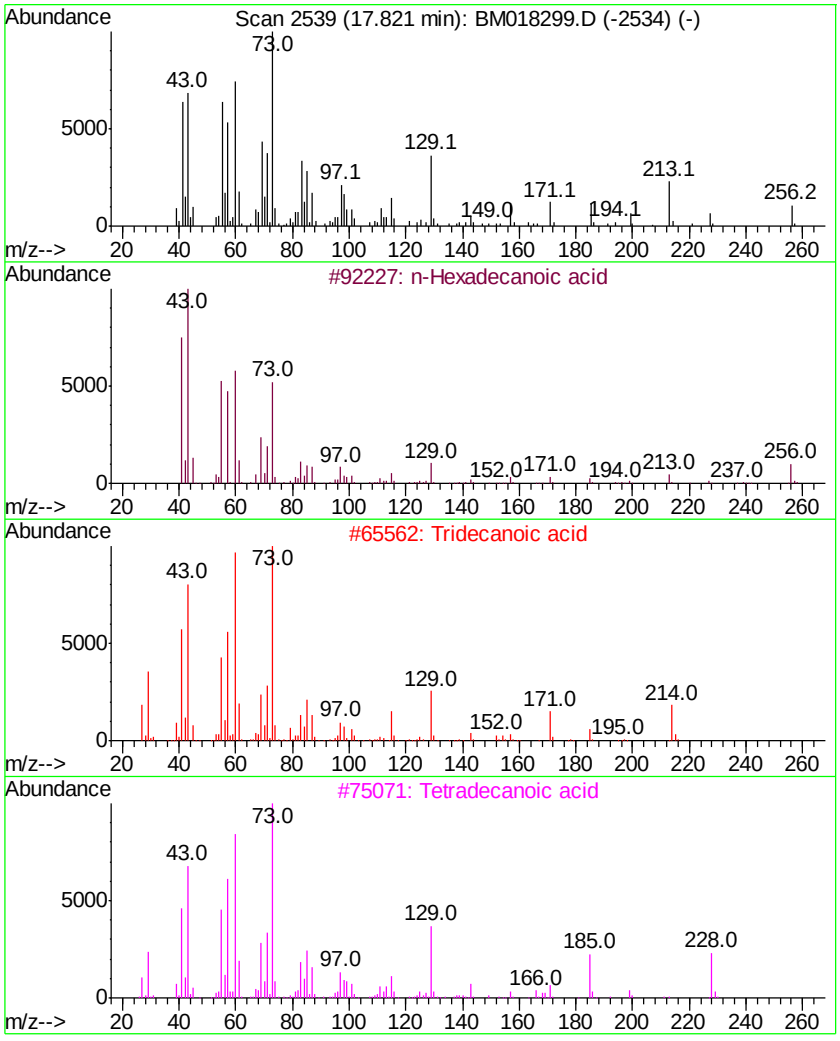
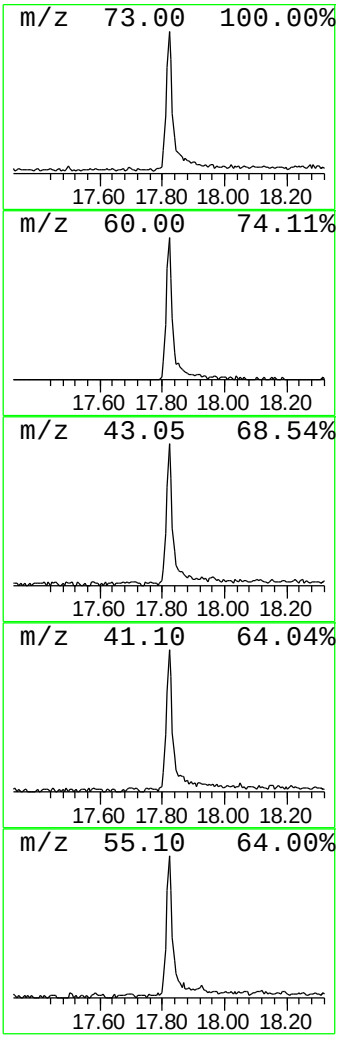
Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.82	8.50 ng	473141	Phenanthrene-d10	16.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Tridecanoic acid	214	C13H26O2	000638-53-9	70
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
4	Undecanoic acid	186	C11H22O2	000112-37-8	47
5	Nonanoic acid	158	C9H18O2	000112-05-0	43





Library Search Compound Report

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Acq On : 19 Dec 2018 15:44
Operator : JU/SJ
Sample : J6446-20
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P001-SS023-1218-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM121518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

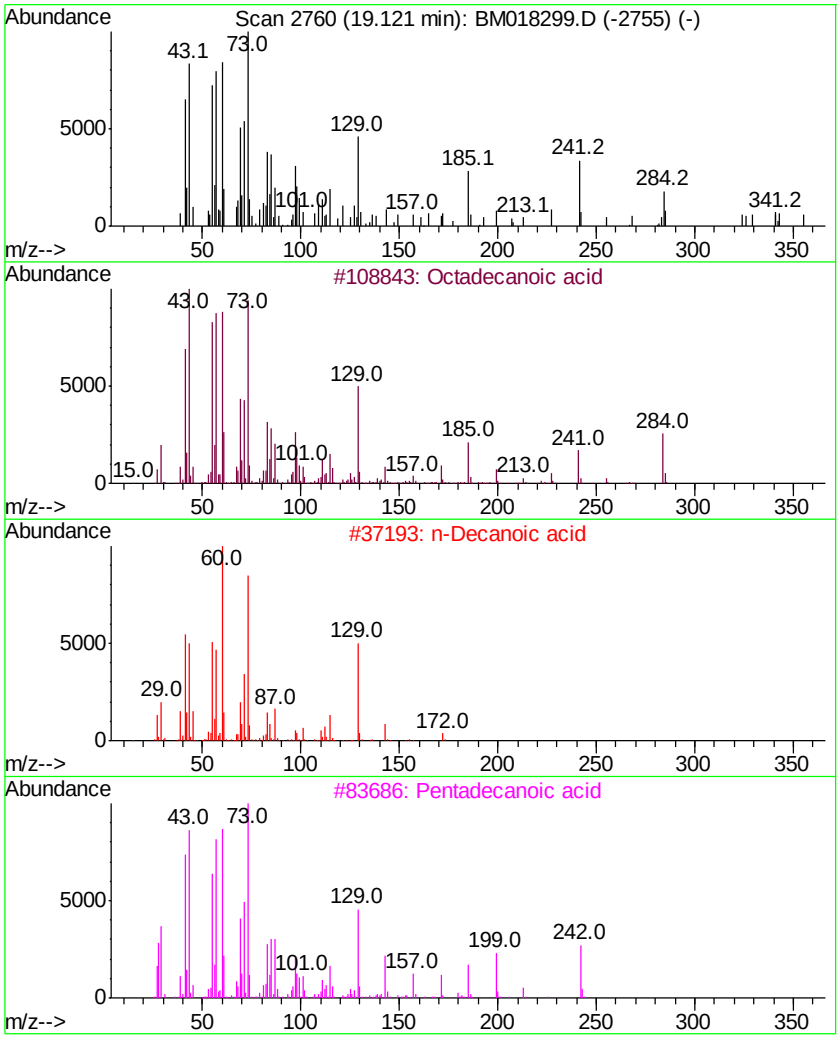
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

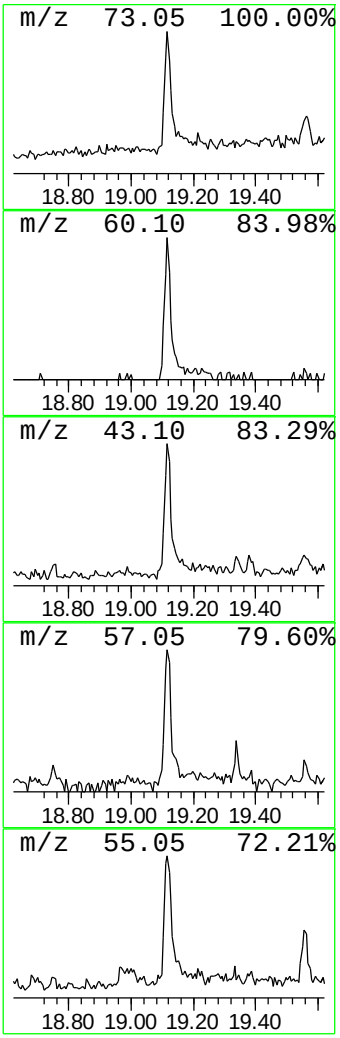
****

Peak Number 5 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.12	2.34 ng	183297	Chrysene-d12	21.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2	n-Decanoic acid	172	C10H20O2	000334-48-5	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5	Tridecanoic acid	214	C13H26O2	000638-53-9	53





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121918\
Data File : BM018299.D
Acq On : 19 Dec 2018 15:44
Operator : JU/SJ
Sample : J6446-20
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P001-SS023-1218-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM121518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

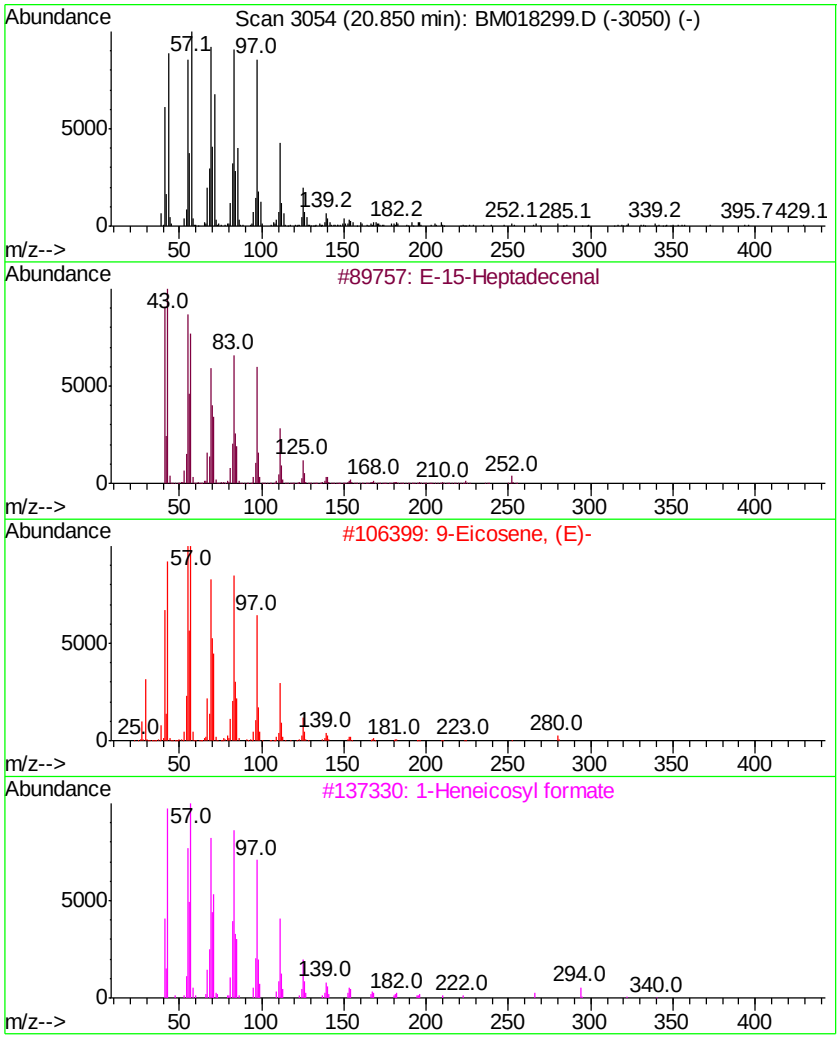
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

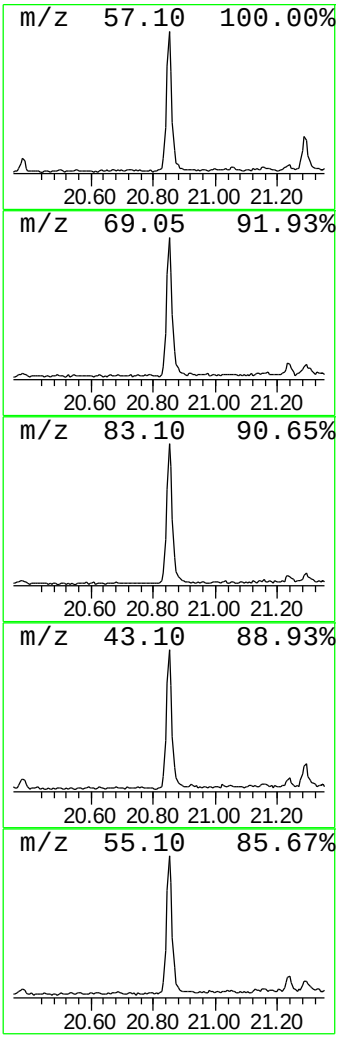
****

Peak Number 6 E-15-Heptadecenal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.85	9.47 ng	740717	Chrysene-d12	21.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-15-Heptadecenal	252	C17H32O	1000130-97-9	93
2	9-Eicosene, (E)-	280	C20H40	074685-29-3	93
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	91
4	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91





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ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM121518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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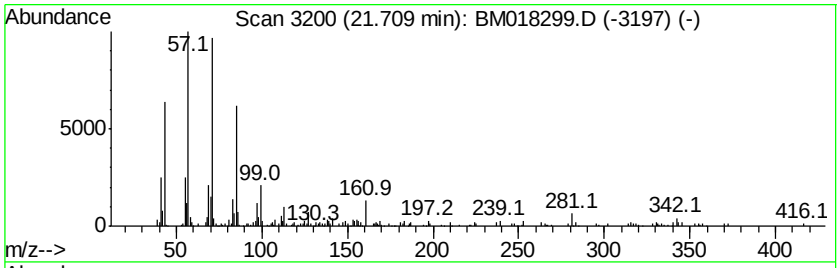
TIC Integration Parameters: LSCINT.P

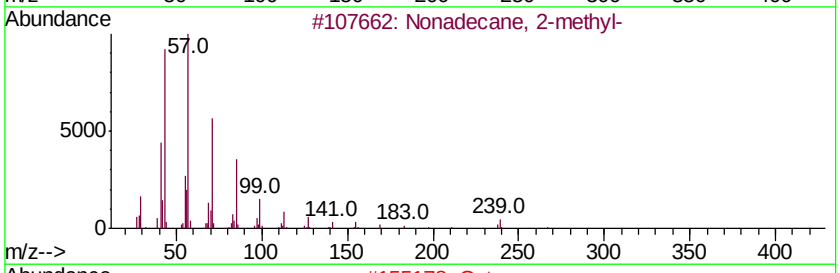
****

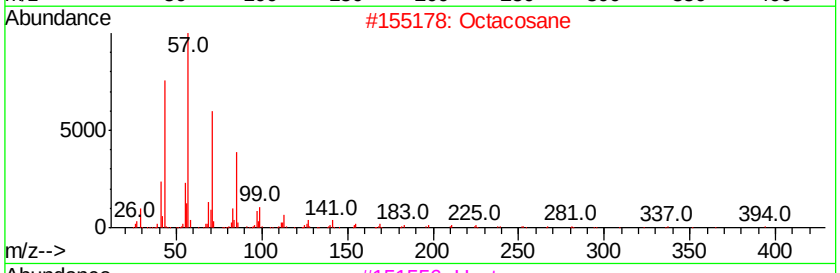
Peak Number 7 Nonadecane, 2-methyl- Concentration Rank 9

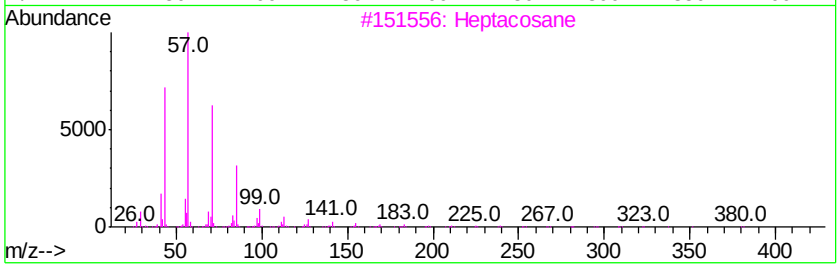
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.71	2.55 ng	199825	Chrysene-d12	21.13

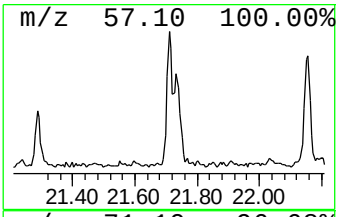
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	80
2	Octacosane	394	C28H58	000630-02-4	74
3	Heptacosane	380	C27H56	000593-49-7	74
4	Tetradecane	198	C14H30	000629-59-4	72
5	Tridecane, 2-methyl-	198	C14H30	001560-96-9	72

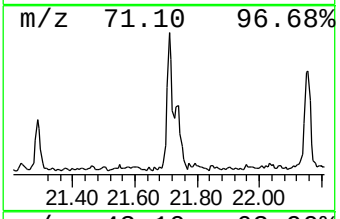


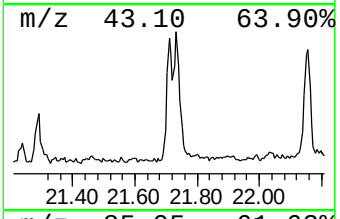


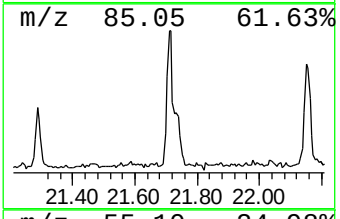


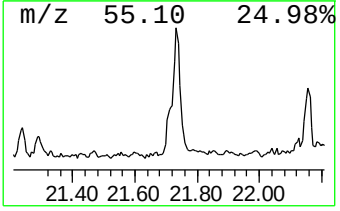












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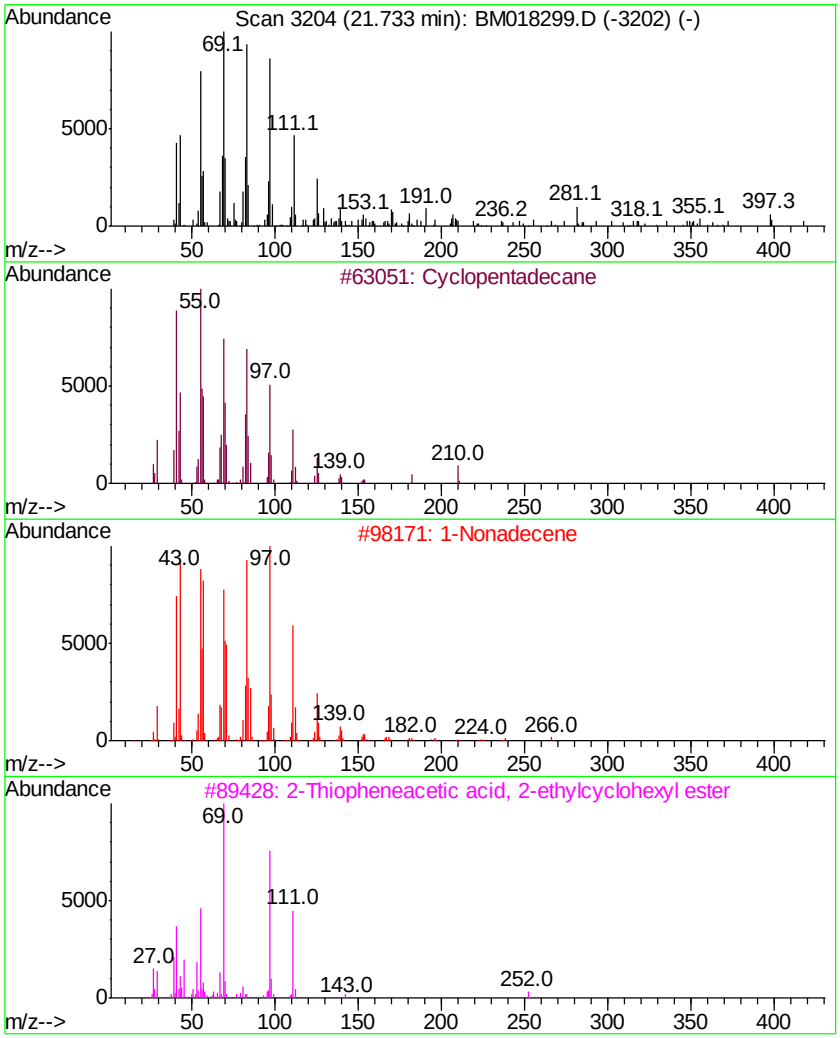
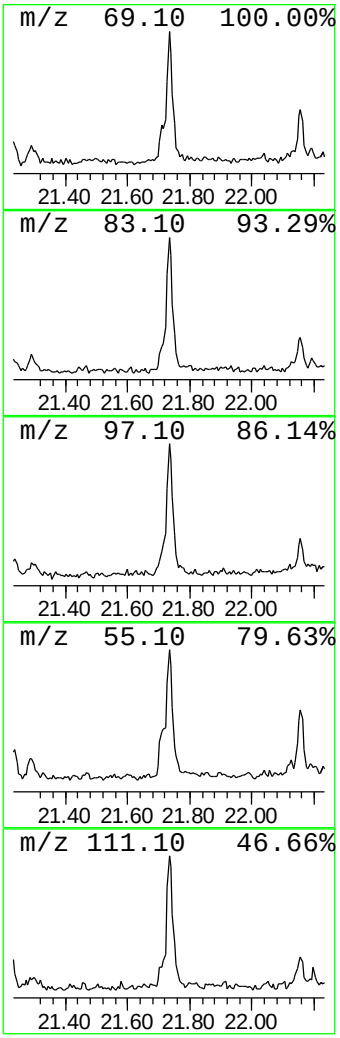
****

Peak Number 8 Cyclopentadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.73	5.25 ng	410890	Chrysene-d12	21.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	87
2	1-Nonadecene	266	C19H38	018435-45-5	59
3	2-Thiopheneacetic acid, 2-ethylc...	252	C14H20O2S	1000278-96-1	43
4	Cyclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	41
5	Cyclohexane, 1,1,2-trimethyl-	126	C9H18	007094-26-0	30





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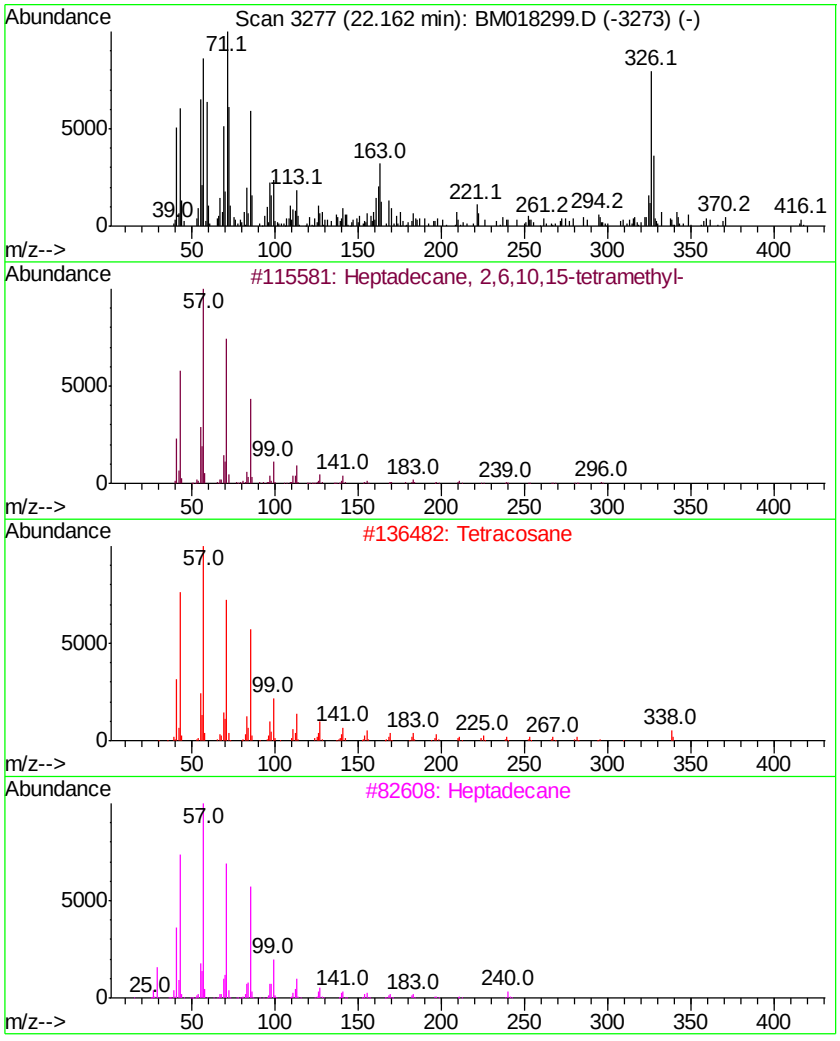
TIC Integration Parameters: LSCINT.P

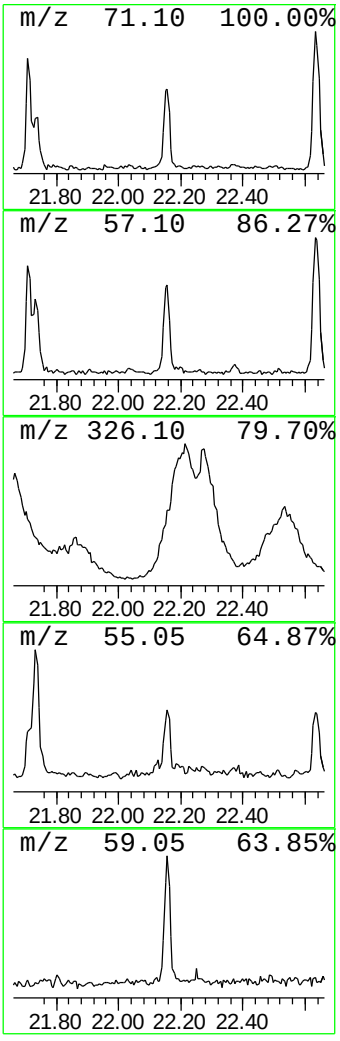
****

Peak Number 9 Heptadecane, 2,6,10,15-tetr... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.16	3.28 ng	256406	Chrysene-d12	21.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86
2	Tetracosane	338	C24H50	000646-31-1	50
3	Heptadecane	240	C17H36	000629-78-7	50
4	Tridecane	184	C13H28	000629-50-5	46
5	Octadecane	254	C18H38	000593-45-3	46





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Data File : BM018299.D
Acq On : 19 Dec 2018 15:44
Operator : JU/SJ
Sample : J6446-20
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P001-SS023-1218-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM121518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

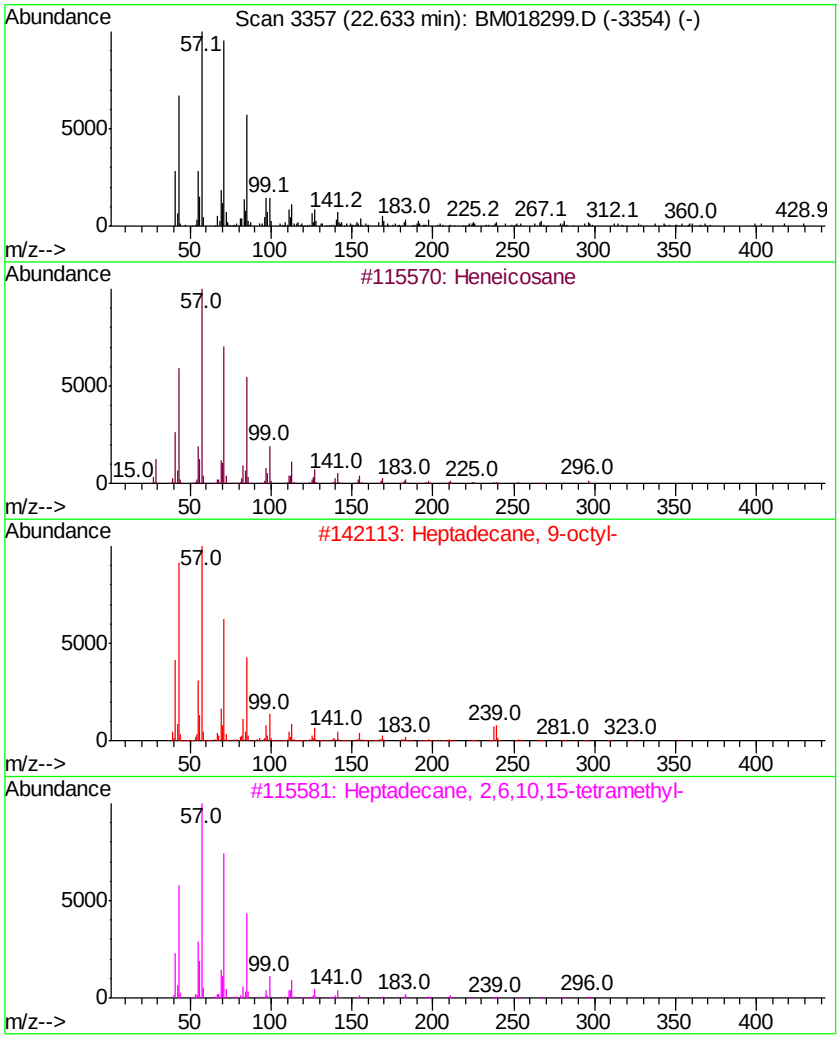
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

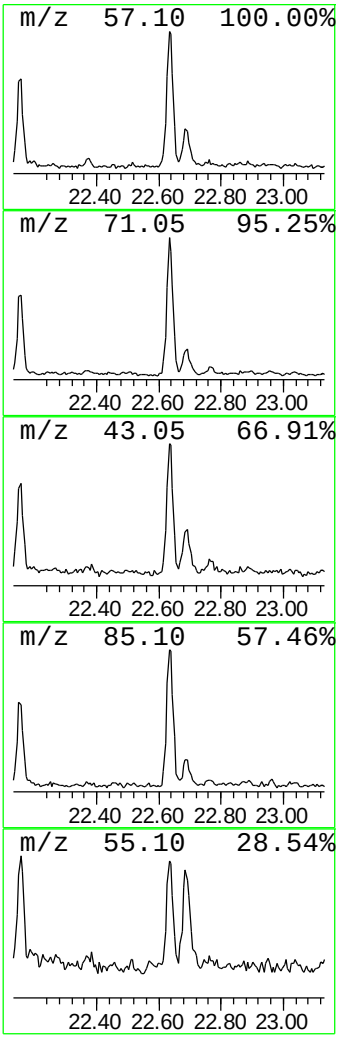
****

Peak Number 10 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.63	3.88 ng	295638	Perylene-d12	23.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	93
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	93
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	93
4	Hexadecane, 5-butyl-	282	C20H42	006912-07-8	91
5	Heptacosane	380	C27H56	000593-49-7	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM121918\
Data File : BM018299.D
Acq On : 19 Dec 2018 15:44
Operator : JU/SJ
Sample : J6446-20
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P001-SS023-1218-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM121518.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
2-Pentanone, 4-hy...	4.68	4.0	ng	120292	1	7.49	595394	20.0
unknown7.03	7.03	108.7	ng	3236210	1	7.49	595394	20.0
n-Hexadecanoic acid	17.82	8.5	ng	473141	4	16.91	1113270	20.0
Octadecanoic acid	19.12	2.3	ng	183297	5	21.13	1564410	20.0
E-15-Heptadecenal	20.85	9.5	ng	740717	5	21.13	1564410	20.0
Nonadecane, 2-met...	21.71	2.5	ng	199825	5	21.13	1564410	20.0
Cyclopentadecane	21.73	5.3	ng	410890	5	21.13	1564410	20.0
Heptadecane, 2,6,...	22.16	3.3	ng	256406	5	21.13	1564410	20.0
Heneicosane	22.63	3.9	ng	295638	6	23.29	1522540	20.0