LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121618\
Data File : BM018235.D
Acq On : 16 Dec 2018 20:20
Operator : JU/SJ
Sample : J6379-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P001-SS003-1824-01

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	3.793	149	154	160	rBV	86960	108503	1.61%	0.220%
2	4.693	302	307	314	rBV	128419	178009	2.64%	0.360%
3	5.134	375	382	400	rBV	3248910	4729513	70.26%	9.569%
4	6.704	641	649	666	rBV	3287407	5522390	82.04%	11.174%
5	7.039	698	706	716	rBV	3461457	5282636	78.48%	10.689%
6	7.498	774	784	791	rBV	542564	841417	12.50%	1.702%
7	7.810	829	837	845	rBV	2590933	3999272	59.41%	8.092%
8	8.657	972	981	993	rBV	1970772	3231776	48.01%	6.539%
9	10.263	1246	1254	1270	rBV	597820	1086080	16.13%	2.198%
10	12.763	1672	1679	1693	rBV	4556395	6731444	100.00%	13.620%
11	13.627	1820	1826	1838	rBV	234326	391779	5.82%	0.793%
12	14.157	1909	1916	1925	rBV2	845461	1330917	19.77%	2.693%
13	15.662	2166	2172	2184	rBV	3117676	4482637	66.59%	9.070%
14	16.915	2379	2385	2398	rBV2	815934	1302018	19.34%	2.634%
15	17.833	2535	2541	2548	rBV	252537	376550	5.59%	0.762%
16	19.127	2757	2761	2768	rBV2	74755	115509	1.72%	0.234%
17	19.574	2830	2837	2843	rBV	4732163	5870933	87.22%	11.879%
18	19.892	2883	2891	2895	rBV3	37771	69814	1.04%	0.141%
19	20.392	2972	2976	2980	rVB	79693	91474	1.36%	0.185%
20	20.862	3051	3056	3065	rBV	418008	559294	8.31%	1.132%
21	21.139	3098	3103	3115	rBV	881737	1246124	18.51%	2.521%
22	21.297	3127	3130	3134	rBV2	114083	121913	1.81%	0.247%
23	21.721	3199	3202	3205	rBV2	116466	145181	2.16%	0.294%
24	22.168	3274	3278	3283	rBV	195228	242760	3.61%	0.491%
25	22.650	3356	3360	3364	rVB2	104691	134315	2.00%	0.272%
26	23.297	3464	3470	3480	rVB2	659355	1231076	18.29%	2.491%

Sum of corrected areas: 49423334

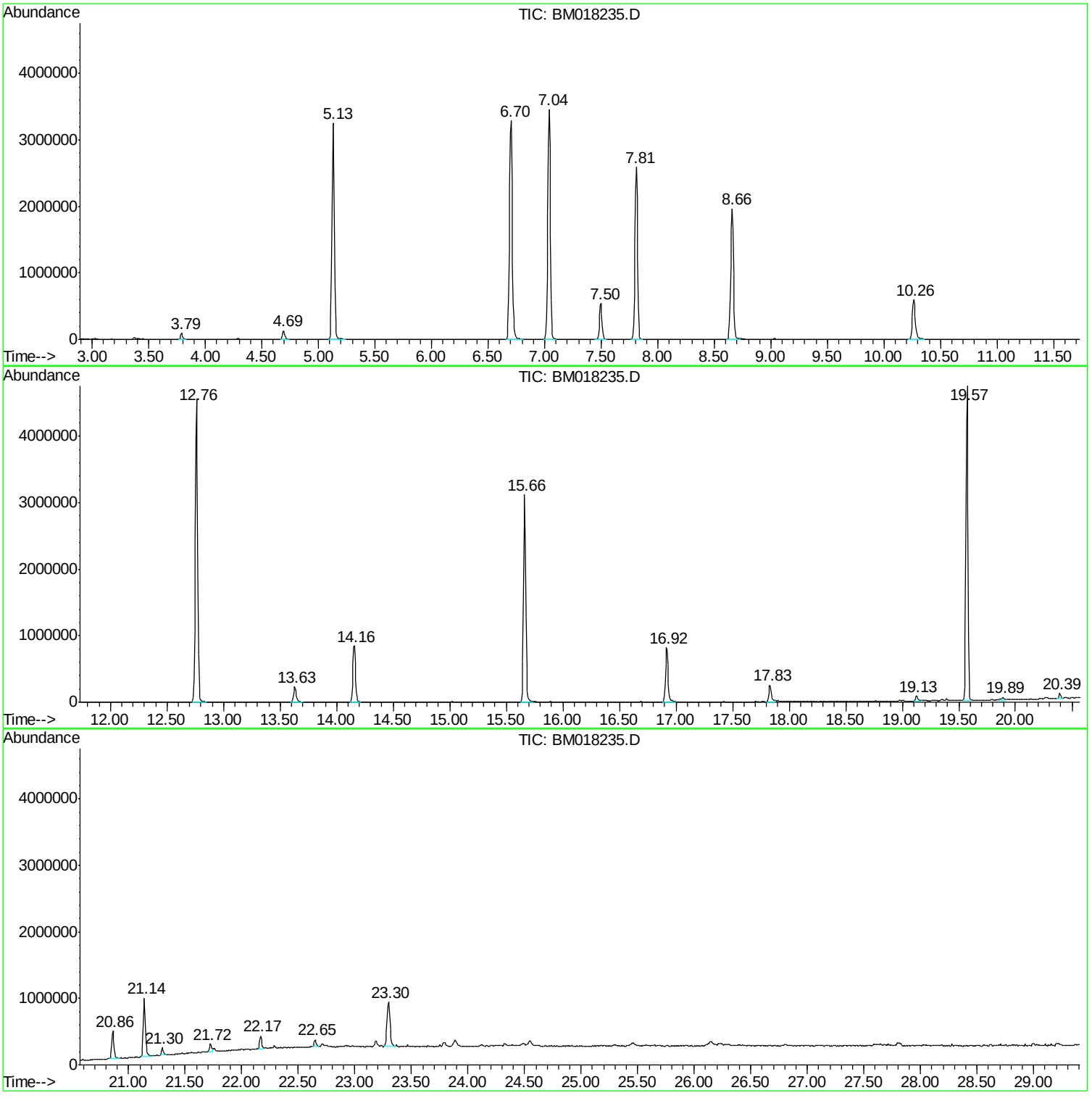
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121618\
Data File : BM018235.D
Acq On : 16 Dec 2018 20:20
Operator : JU/SJ
Sample : J6379-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P001-SS003-1824-01

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121618\
Data File : BM018235.D
Acq On : 16 Dec 2018 20:20
Operator : JU/SJ
Sample : J6379-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P001-SS003-1824-01

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

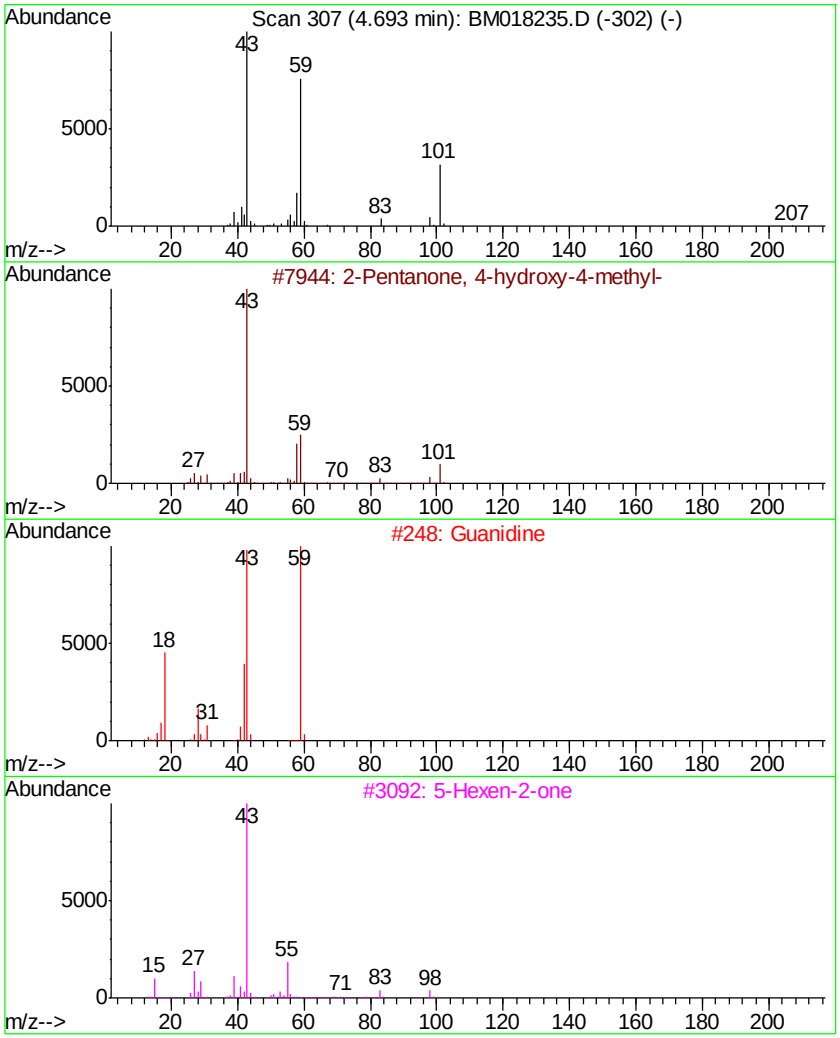
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

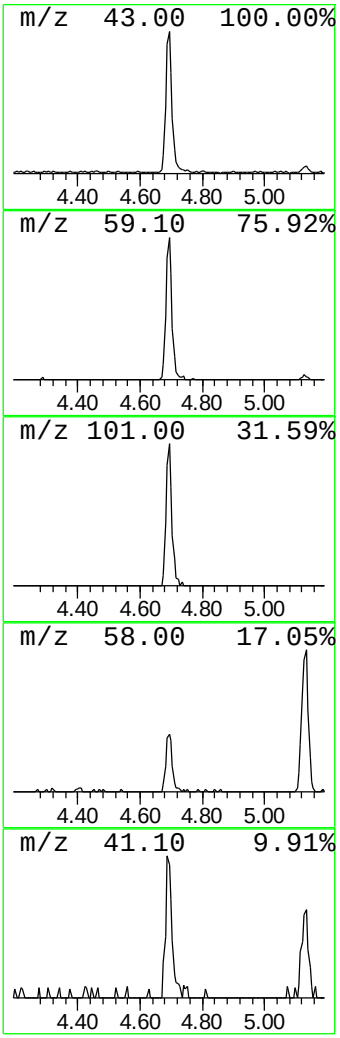
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.69	4.23 ng	178009	1,4-Dichlorobenzene-d4	7.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Guanidine	59	CH5N3	000113-00-8	50
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121618\
Data File : BM018235.D
Acq On : 16 Dec 2018 20:20
Operator : JU/SJ
Sample : J6379-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P001-SS003-1824-01

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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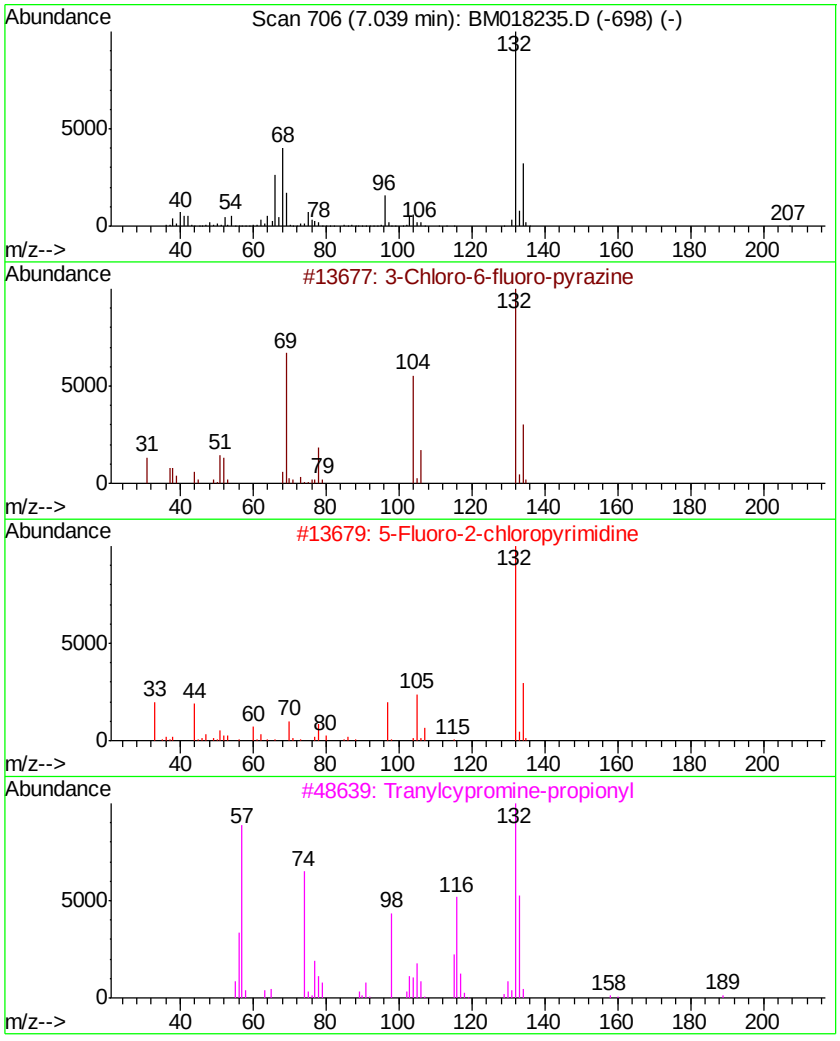
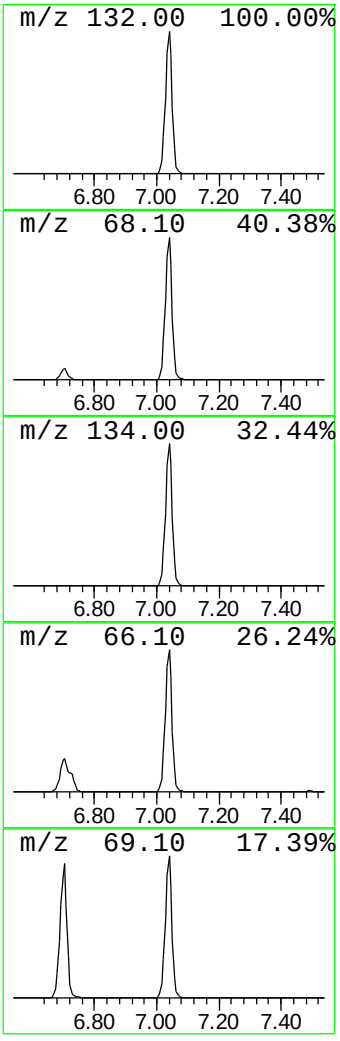
Peak Number 3 unknown7.04 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.04	125.57 ng	5282640	1,4-Dichlorobenzene-d4	7.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121618\
Data File : BM018235.D
Acq On : 16 Dec 2018 20:20
Operator : JU/SJ
Sample : J6379-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P001-SS003-1824-01

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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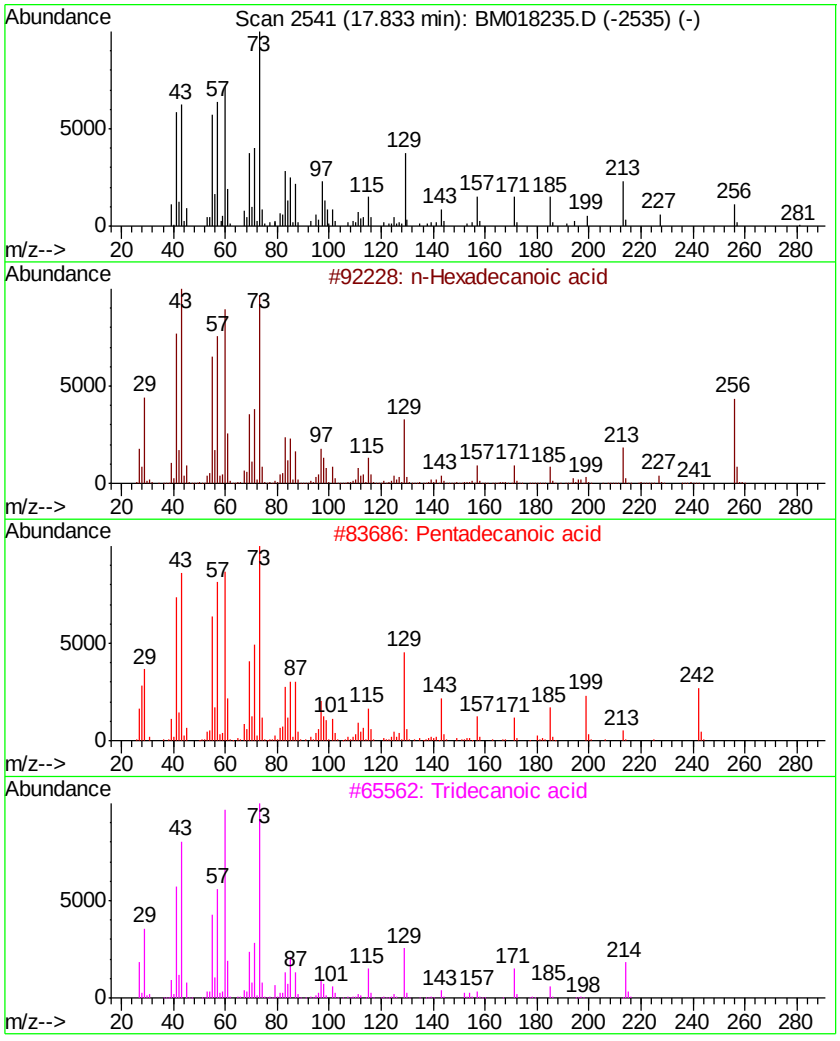
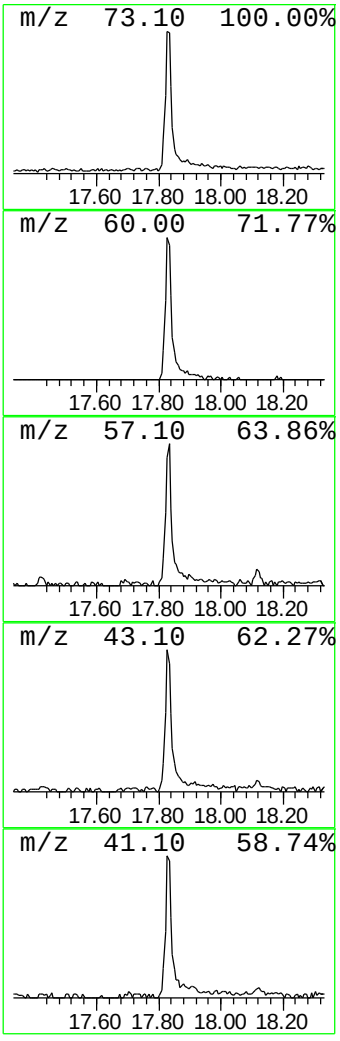
Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.83	5.78 ng	376550	Phenanthrene-d10	16.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Tridecanoic acid	214	C13H26O2	000638-53-9	64
4	n-Decanoic acid	172	C10H20O2	000334-48-5	64
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	46





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121618\
Data File : BM018235.D
Acq On : 16 Dec 2018 20:20
Operator : JU/SJ
Sample : J6379-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P001-SS003-1824-01

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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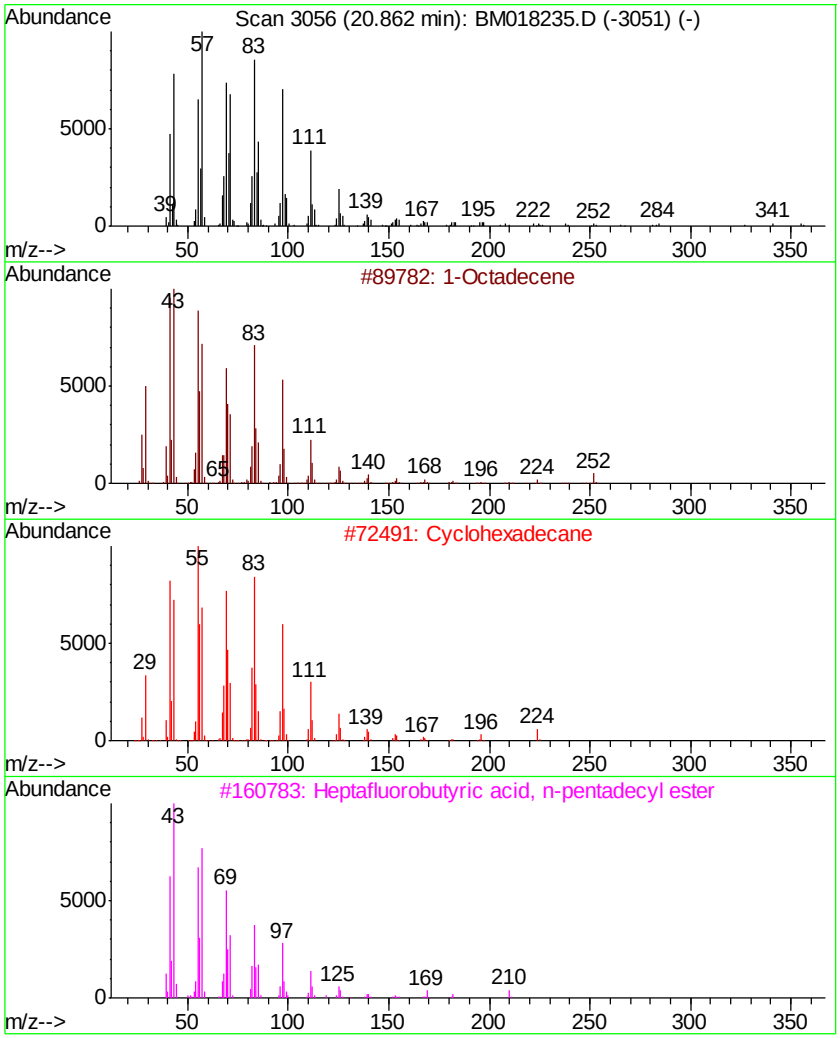
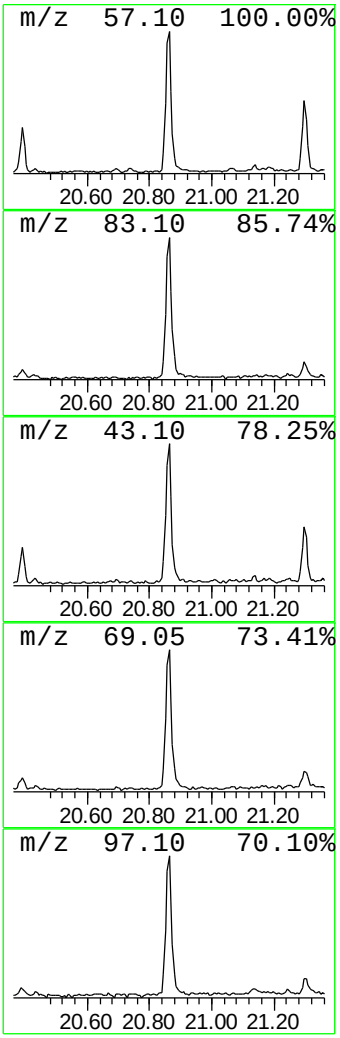
Peak Number 6 1-Octadecene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.86	8.98 ng	559294	Chrysene-d12	21.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene	252	C18H36	000112-88-9	91
2	Cyclohexadecane	224	C16H32	000295-65-8	90
3	Heptafluorobutyric acid, n-penta...	424	C19H31F7O2	1000216-79-3	87
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121618\
Data File : BM018235.D
Acq On : 16 Dec 2018 20:20
Operator : JU/SJ
Sample : J6379-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P001-SS003-1824-01

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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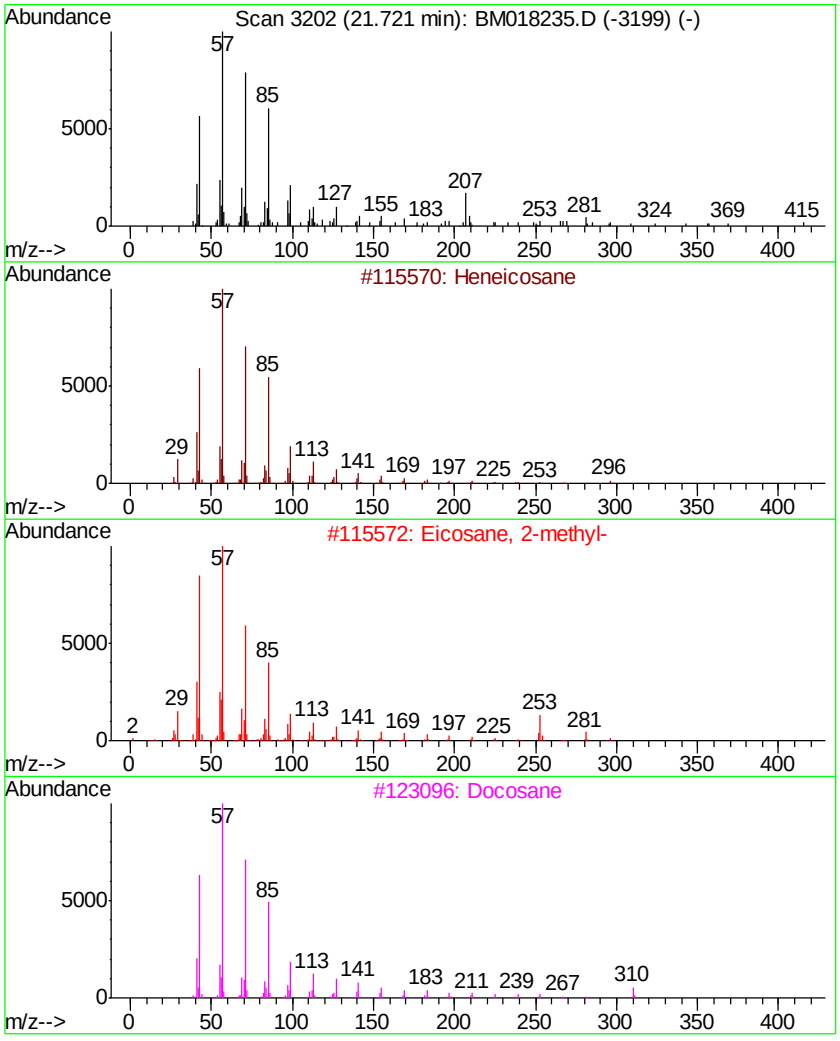
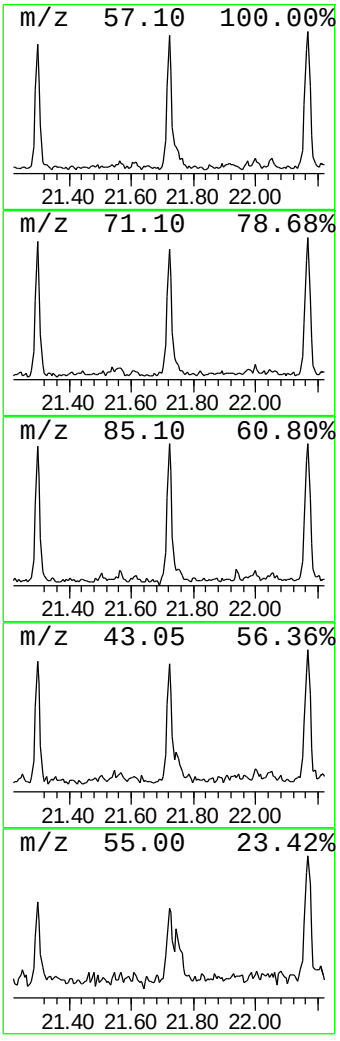
Peak Number 7 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.72	2.33 ng	145181	Chrysene-d12	21.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	98
2	Eicosane, 2-methyl-	296	C21H44	001560-84-5	93
3	Docosane	310	C22H46	000629-97-0	83
4	Triacontane	422	C30H62	000638-68-6	83
5	Heptacosane	380	C27H56	000593-49-7	83





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121618\
Data File : BM018235.D
Acq On : 16 Dec 2018 20:20
Operator : JU/SJ
Sample : J6379-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P001-SS003-1824-01

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

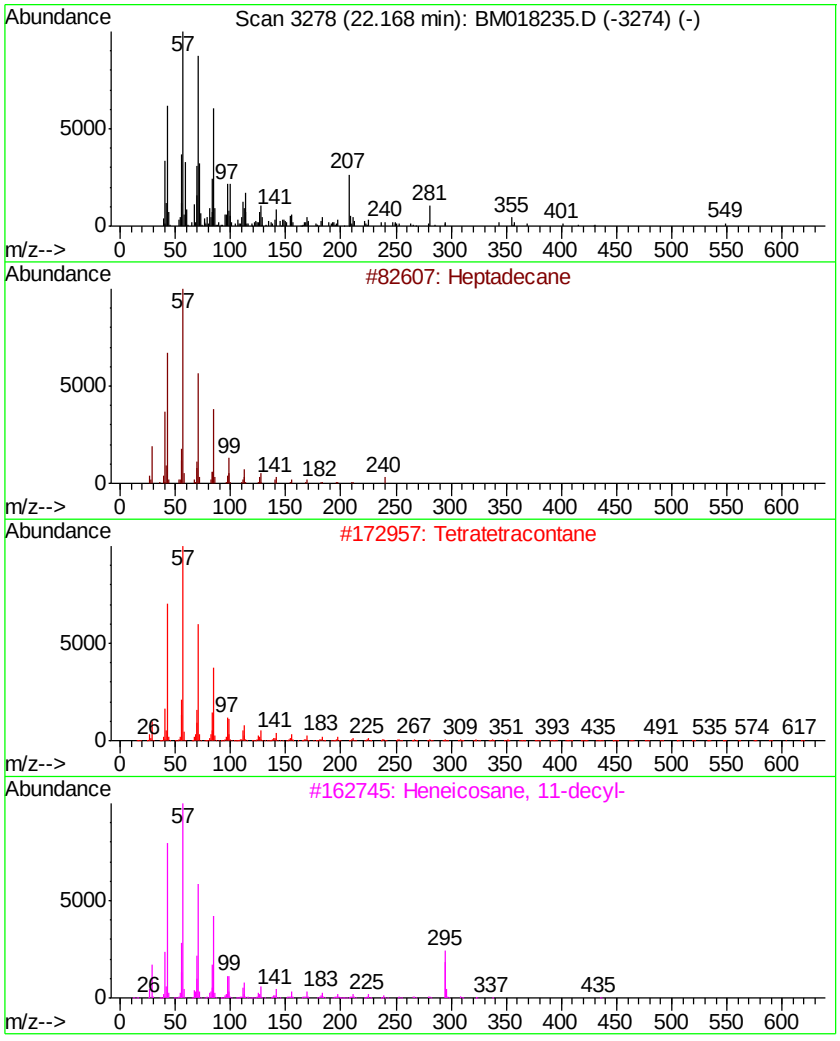
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

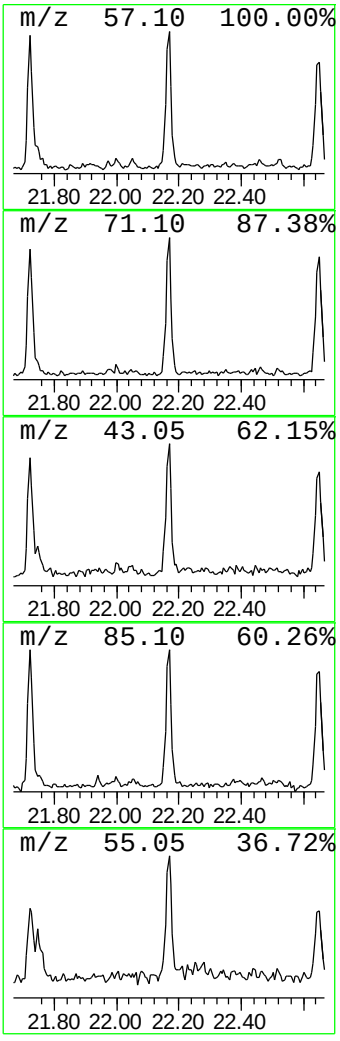
****

Peak Number 8 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.17	3.90 ng	242760	Chrysene-d12	21.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	83
2	Tetratetracontane	619	C44H90	007098-22-8	64
3	Heneicosane, 11-decyl-	437	C31H64	055320-06-4	64
4	Tetratriacontane	479	C34H70	014167-59-0	62
5	Triacontane, 1-bromo-	500	C30H61Br	004209-22-7	62





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121618\
Data File : BM018235.D
Acq On : 16 Dec 2018 20:20
Operator : JU/SJ
Sample : J6379-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P001-SS003-1824-01

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

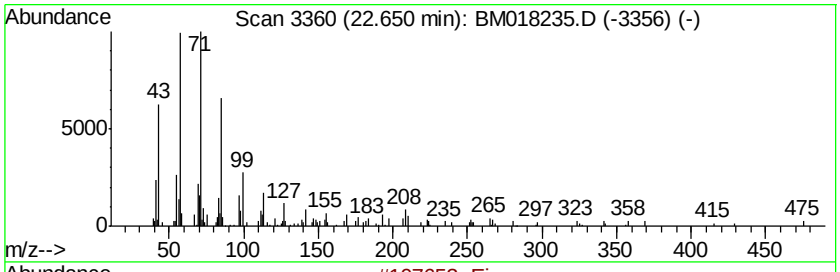
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

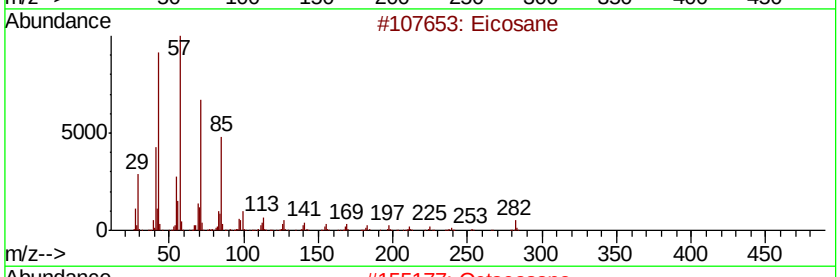
****

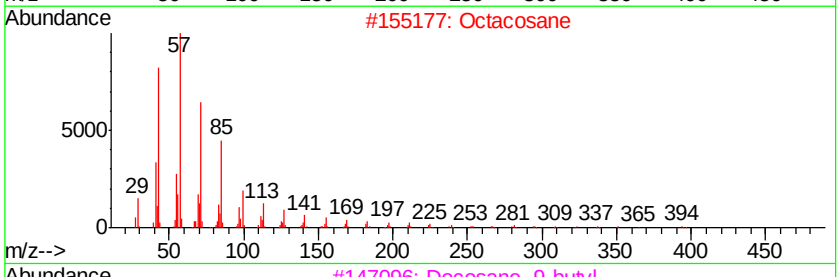
Peak Number 9 Eicosane Concentration Rank 9

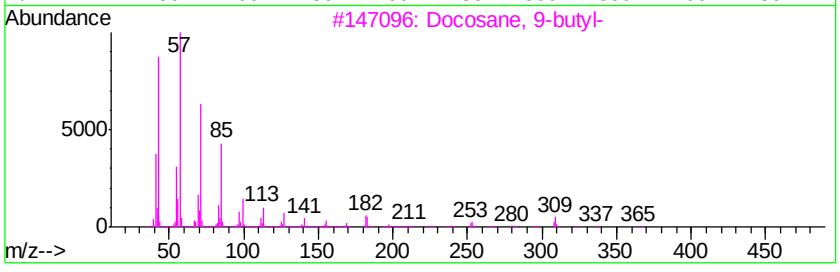
R.T.	EstConc	Area	Relative to ISTD	R.T.
22.65	2.18 ng	134315	Perylene-d12	23.30

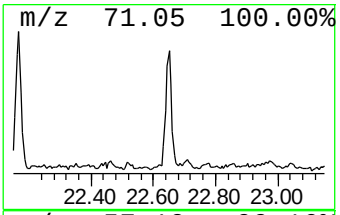
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	89
2	Octacosane	394	C28H58	000630-02-4	80
3	Docosane, 9-butyl-	366	C26H54	055282-14-9	80
4	Tetracosane	338	C24H50	000646-31-1	80
5	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	80

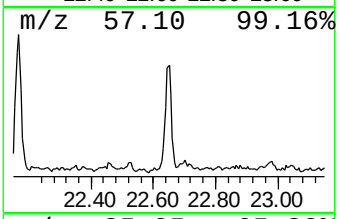


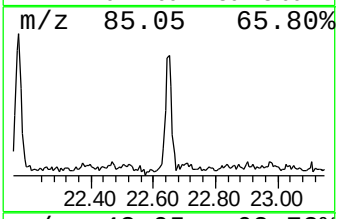


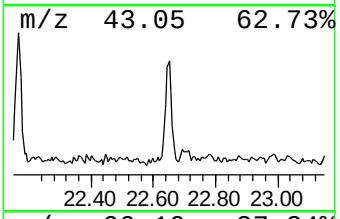


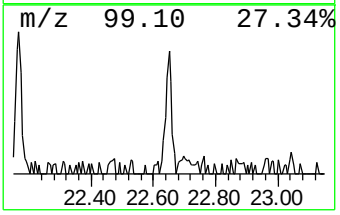












Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM121618\
Data File : BM018235.D
Acq On : 16 Dec 2018 20:20
Operator : JU/SJ
Sample : J6379-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P001-SS003-1824-01

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...	4.69	4.2	ng	178009	1	7.50	841417	20.0
unknown7.04	7.04	125.6	ng	5282640	1	7.50	841417	20.0
n-Hexadecanoic acid	17.83	5.8	ng	376550	4	16.92	1302020	20.0
1-Octadecene	20.86	9.0	ng	559294	5	21.14	1246120	20.0
Heneicosane	21.72	2.3	ng	145181	5	21.14	1246120	20.0
Heptadecane	22.17	3.9	ng	242760	5	21.14	1246120	20.0
Eicosane	22.65	2.2	ng	134315	6	23.30	1231080	20.0