LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM010919\
Data File : BM018475.D
Acq On : 09 Jan 2019 16:28
Operator : JU/SJ
Sample : K1088-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CPSB-05(10-15)

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-BM010919.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	4.899	303	308	318	rVB	385706	555893	1.81%	0.310%
2	5.352	378	385	397	rBV	9168247	12928061	42.18%	7.213%
3	6.940	647	655	665	rBV	8744803	14192373	46.31%	7.918%
4	7.299	707	716	728	rBV	9461051	14968025	48.84%	8.351%
5	7.763	787	795	801	rBV	1774525	2865902	9.35%	1.599%
6	8.081	841	849	858	rVB	7037073	11240712	36.68%	6.271%
7	8.928	984	993	1005	rBV	5325478	8717762	28.44%	4.864%
8	10.551	1262	1269	1280	rVB	2292735	3757588	12.26%	2.096%
9	13.028	1682	1690	1699	rBV	13815637	20282175	66.17%	11.316%
10	13.863	1825	1832	1841	rBV	1251721	1795896	5.86%	1.002%
11	14.410	1917	1925	1934	rVB2	3134555	4900051	15.99%	2.734%
12	15.904	2171	2179	2196	rBV	10880800	15883142	51.82%	8.861%
13	17.157	2386	2392	2399	rBV2	4262947	6014312	19.62%	3.355%
14	18.051	2537	2544	2566	rBV	3143911	5542411	18.08%	3.092%
15	19.216	2734	2742	2749	rBV3	253812	650948	2.12%	0.363%
16	19.333	2756	2762	2786	rBV	3921421	6518673	21.27%	3.637%
17	19.792	2834	2840	2846	rBV	25670583	30649400	100.00%	17.100%
18	21.057	3051	3055	3064	rBV	1168429	1540295	5.03%	0.859%
19	21.351	3100	3105	3111	rBV	5725126	7084002	23.11%	3.952%
20	21.939	3202	3205	3211	rBV2	267430	370778	1.21%	0.207%
21	22.410	3282	3285	3292	rVB2	490183	621414	2.03%	0.347%
22	22.539	3305	3307	3314	rVB	290945	339432	1.11%	0.189%
23	22.927	3369	3373	3378	rVB	478906	675272	2.20%	0.377%
24	23.509	3468	3472	3481	rVB	439571	740633	2.42%	0.413%
25	23.639	3488	3494	3505	rVB	3327966	6405226	20.90%	3.574%

Sum of corrected areas: 179240376

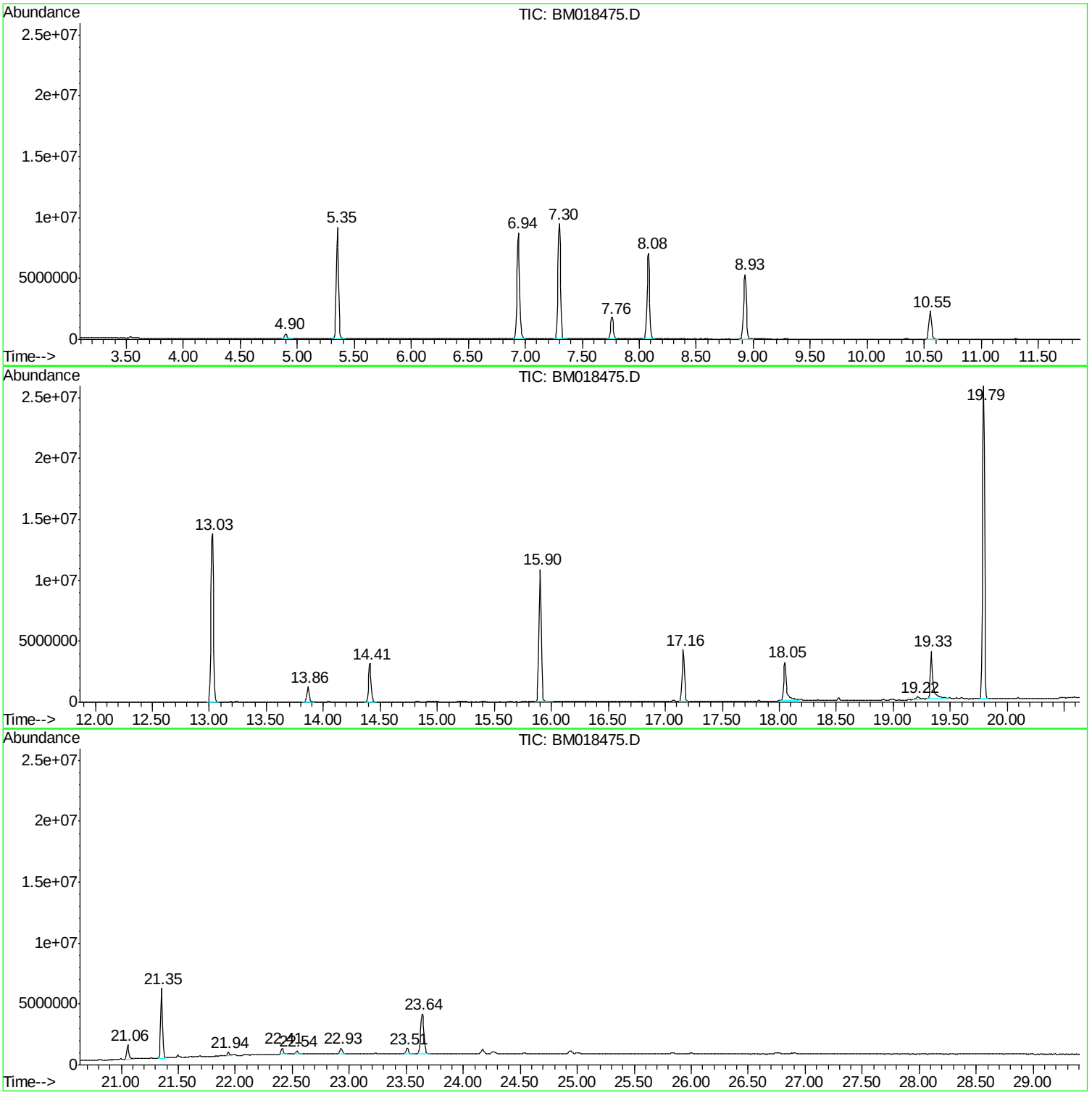
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM010919\
Data File : BM018475.D
Acq On : 09 Jan 2019 16:28
Operator : JU/SJ
Sample : K1088-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CPSB-05(10-15)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.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\BM010919\
Data File : BM018475.D
Acq On : 09 Jan 2019 16:28
Operator : JU/SJ
Sample : K1088-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CPSB-05(10-15)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

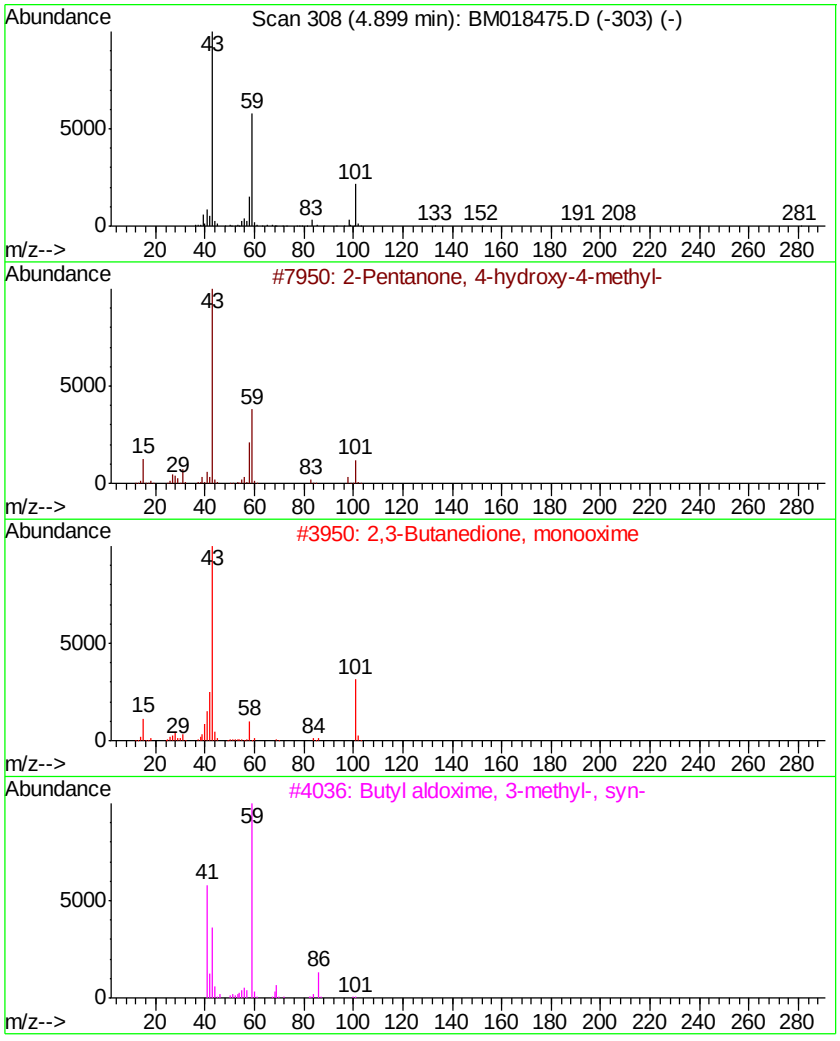
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

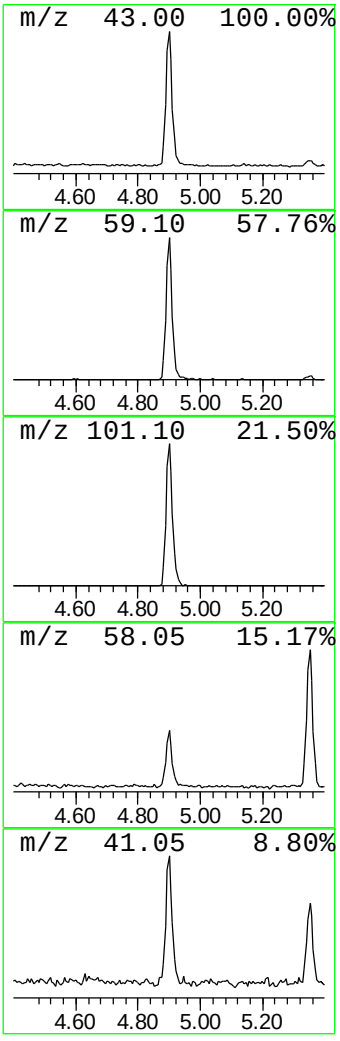
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	3.88 ng	555893	1,4-Dichlorobenzene-d4	7.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	47
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM010919\
Data File : BM018475.D
Acq On : 09 Jan 2019 16:28
Operator : JU/SJ
Sample : K1088-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CPSB-05(10-15)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.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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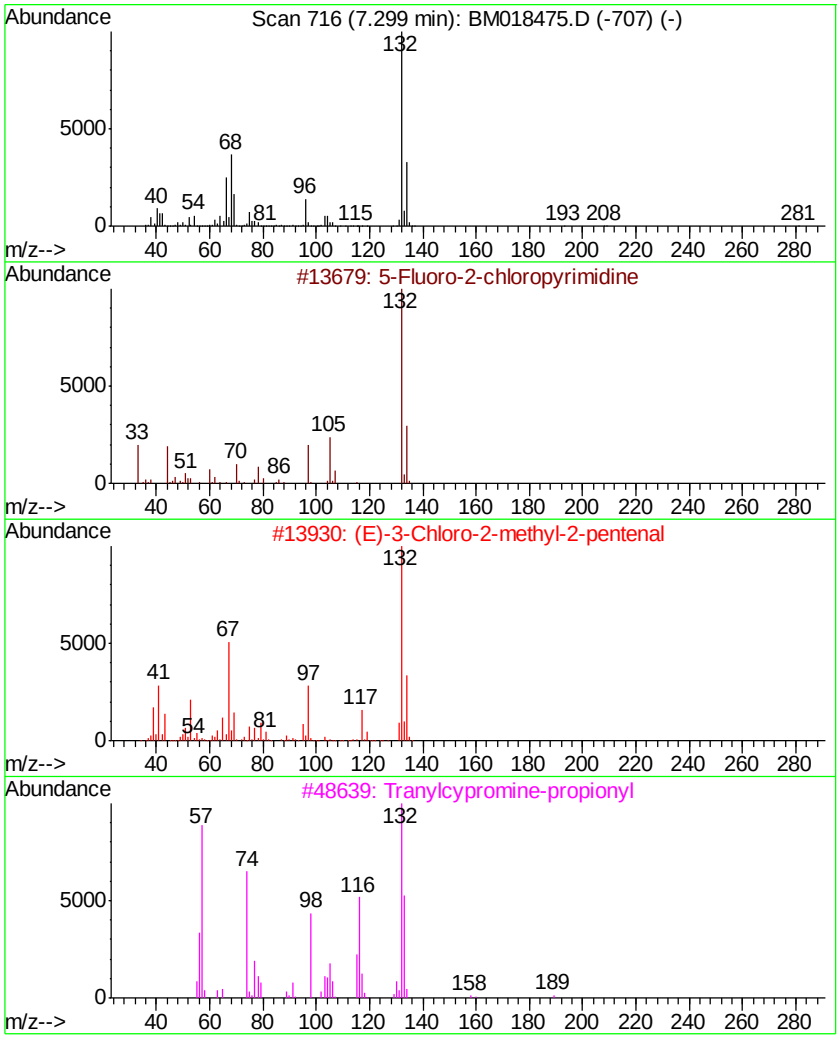
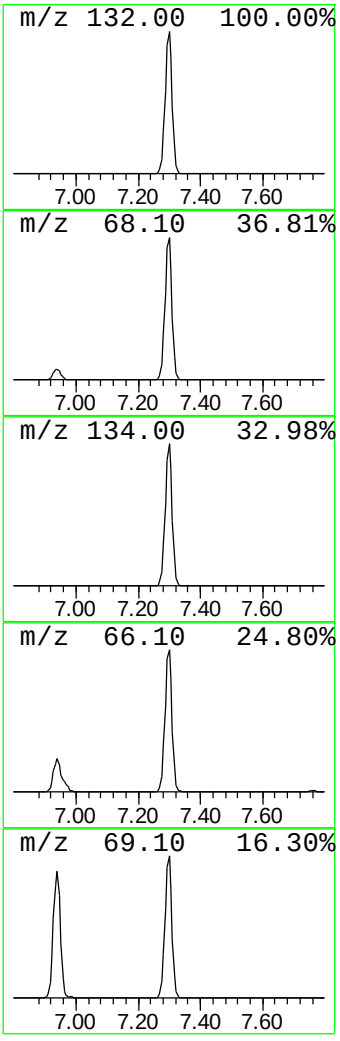
Peak Number 2 unknown7.30 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.30	104.46 ng	14968000	1,4-Dichlorobenzene-d4	7.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	17
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
4	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM010919\
Data File : BM018475.D
Acq On : 09 Jan 2019 16:28
Operator : JU/SJ
Sample : K1088-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CPSB-05(10-15)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.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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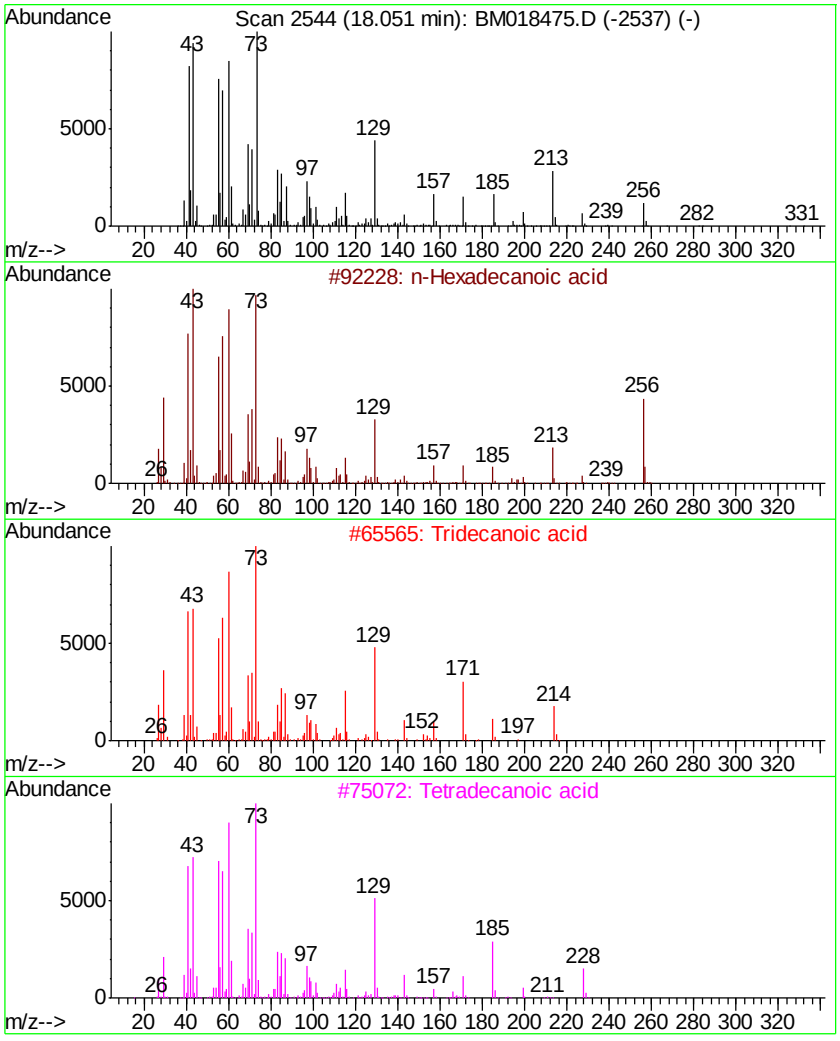
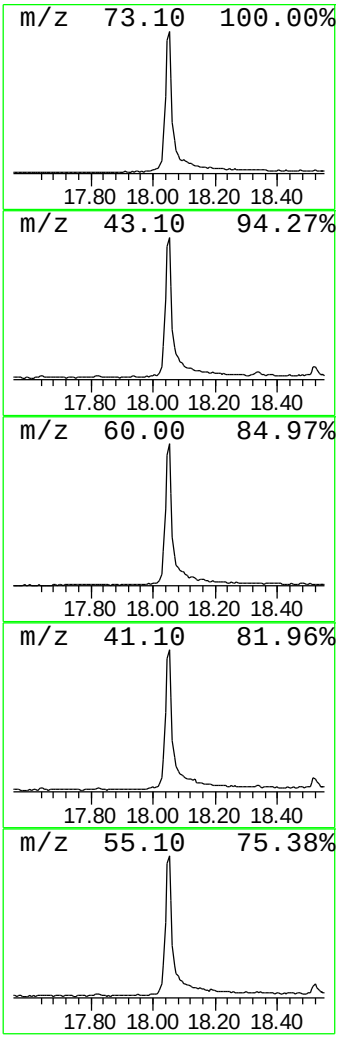
Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.05	18.43 ng	5542410	Phenanthrene-d10	17.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5	Undecanoic acid	186	C11H22O2	000112-37-8	80





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM010919\
Data File : BM018475.D
Acq On : 09 Jan 2019 16:28
Operator : JU/SJ
Sample : K1088-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CPSB-05(10-15)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

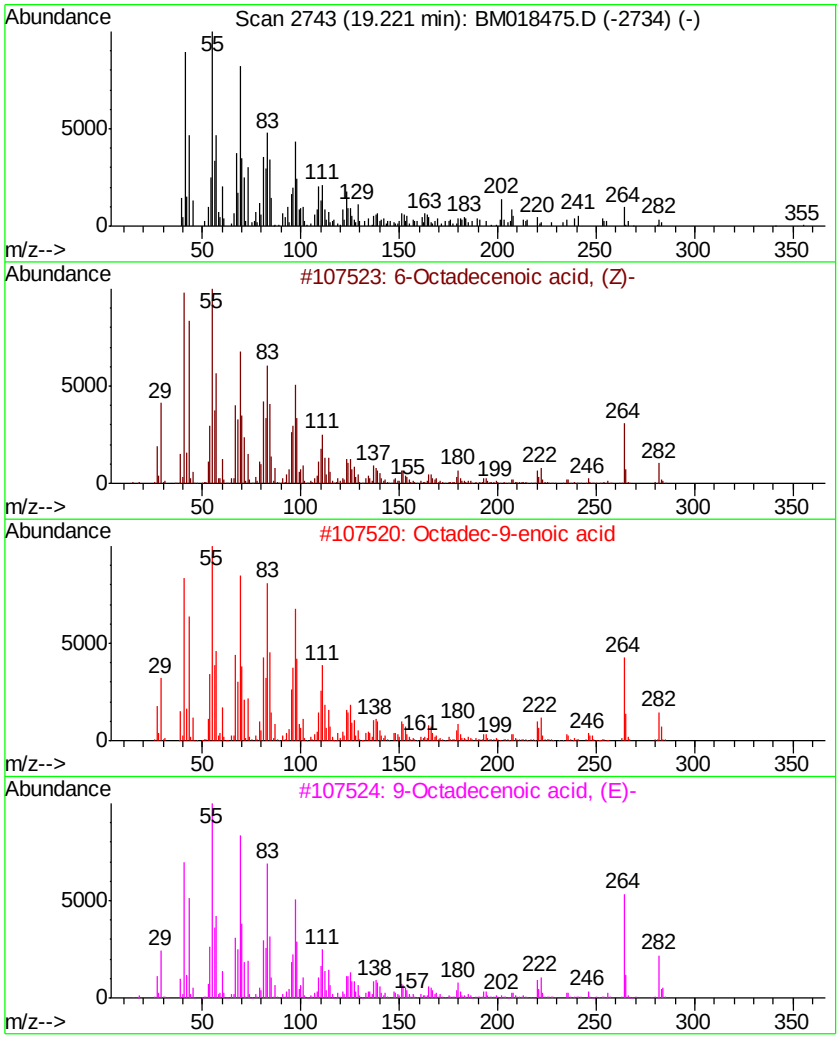
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

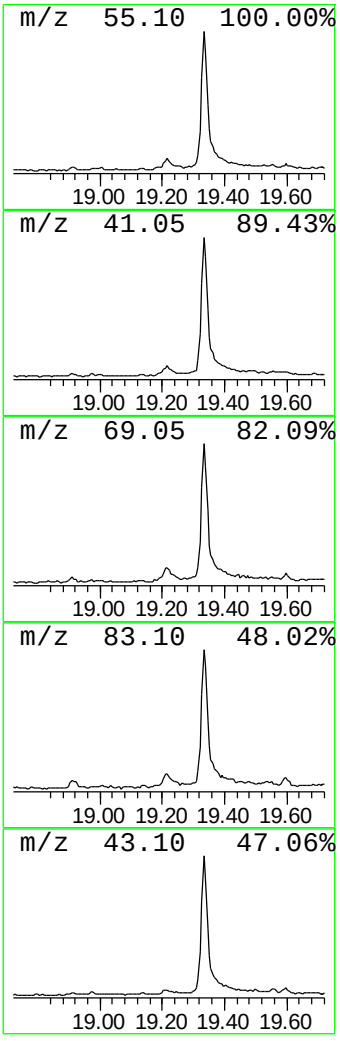
****

Peak Number 5 6-Octadecenoic acid, (Z)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.22	2.16 ng	650948	Phenanthrene-d10	17.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Octadecenoic acid, (Z)-	282	C18H34O2	000593-39-5	97
2	Octadec-9-enoic acid	282	C18H34O2	1000190-13-7	96
3	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	96
4	Oleic Acid	282	C18H34O2	000112-80-1	81
5	9-Hexadecenoic acid	254	C16H30O2	002091-29-4	62





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM010919\
Data File : BM018475.D
Acq On : 09 Jan 2019 16:28
Operator : JU/SJ
Sample : K1088-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CPSB-05(10-15)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

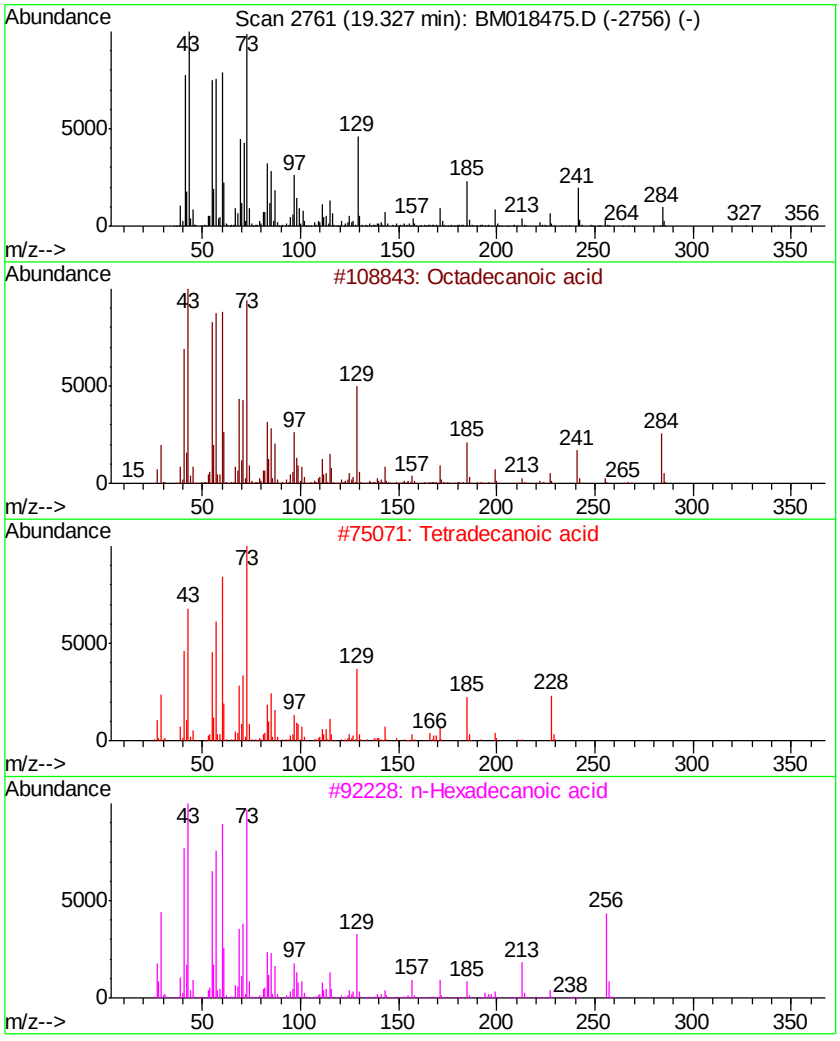
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

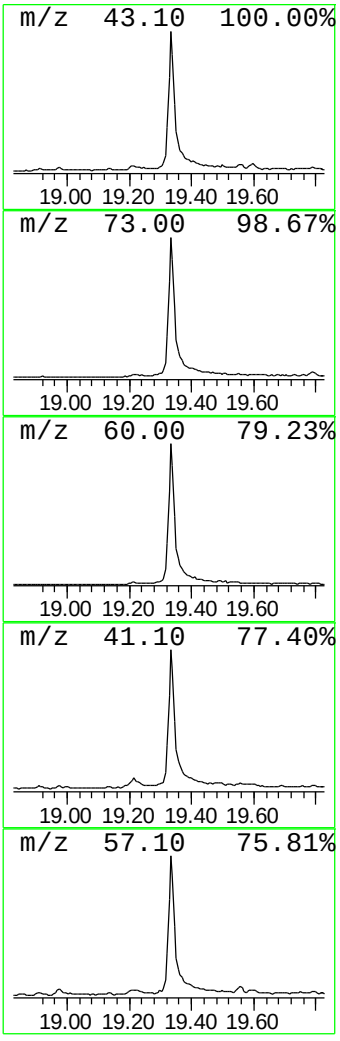
****

Peak Number 6 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.33	18.40 ng	6518670	Chrysene-d12	21.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
5	Tridecanoic acid	214	C13H26O2	000638-53-9	76





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM010919\
Data File : BM018475.D
Acq On : 09 Jan 2019 16:28
Operator : JU/SJ
Sample : K1088-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CPSB-05(10-15)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

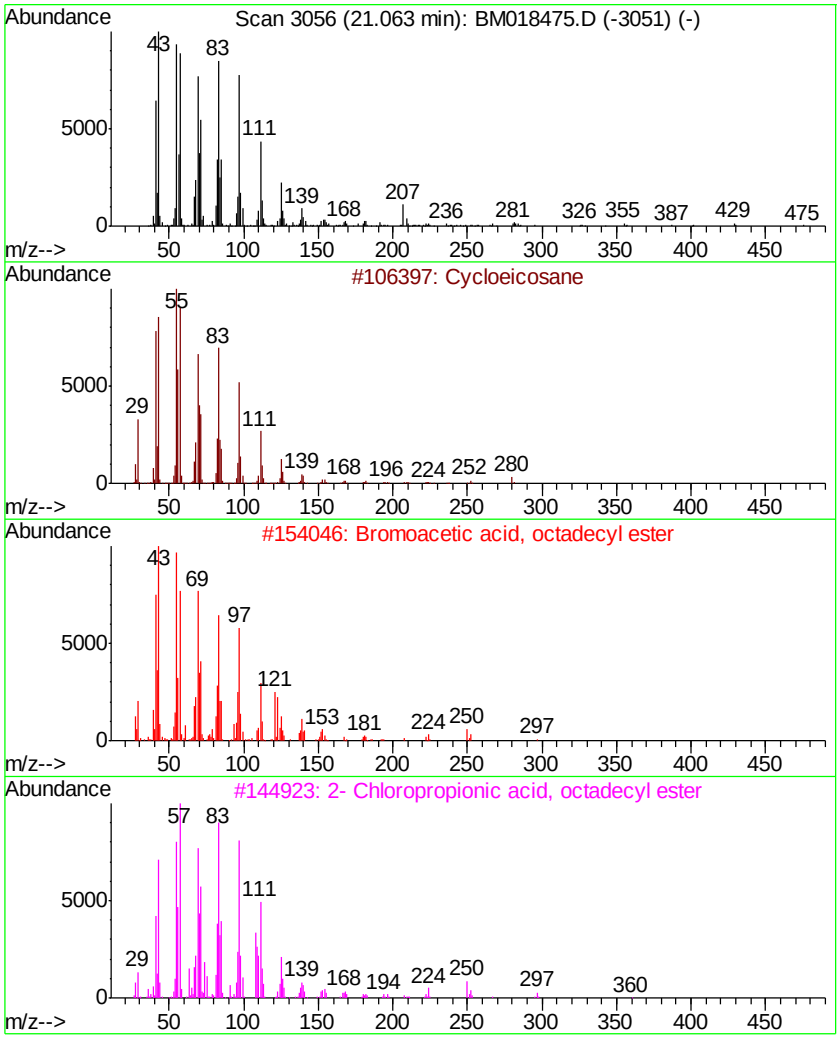
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

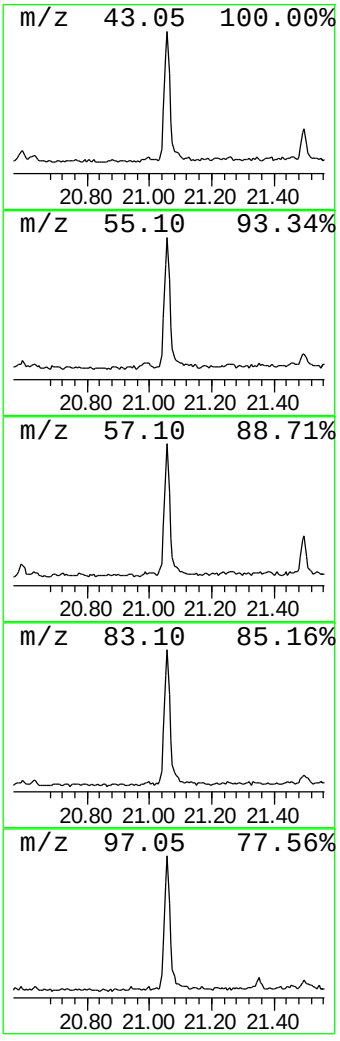
****

Peak Number 7 Cycloeicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.06	4.35 ng	1540300	Chrysene-d12	21.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloeicosane	280	C20H40	000296-56-0	95
2	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
3	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
4	1-Nonadecene	266	C19H38	018435-45-5	91
5	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM010919\
Data File : BM018475.D
Acq On : 09 Jan 2019 16:28
Operator : JU/SJ
Sample : K1088-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CPSB-05(10-15)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

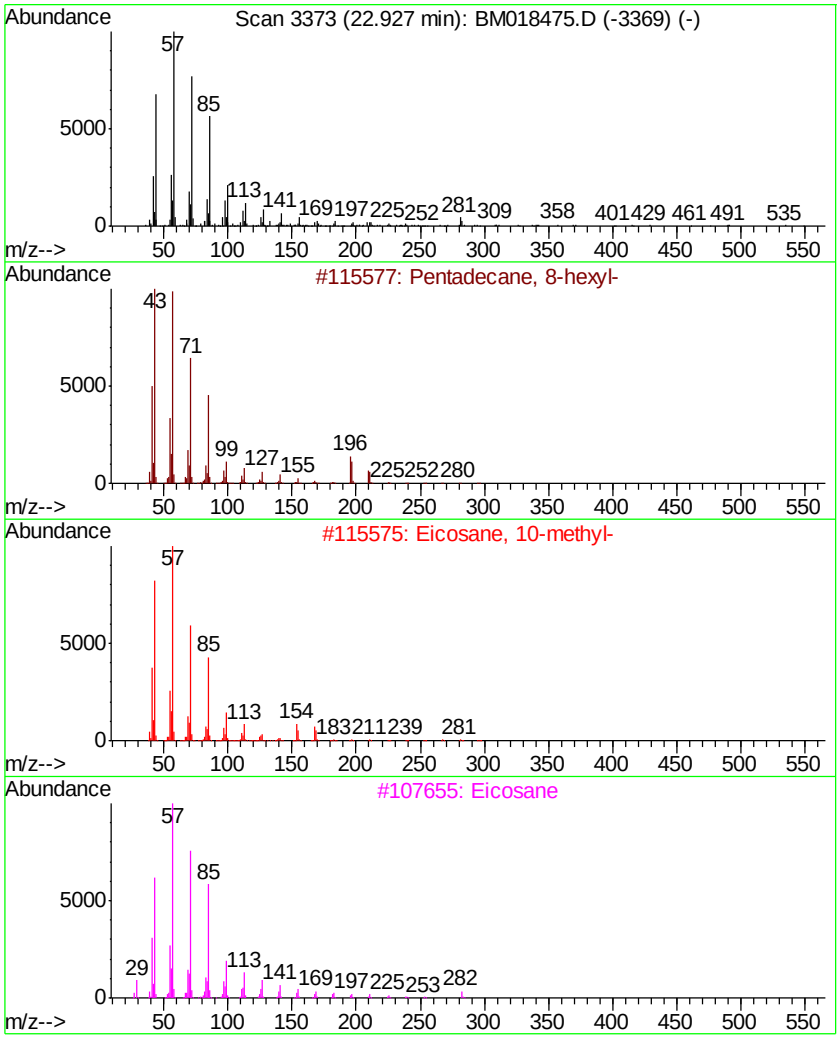
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

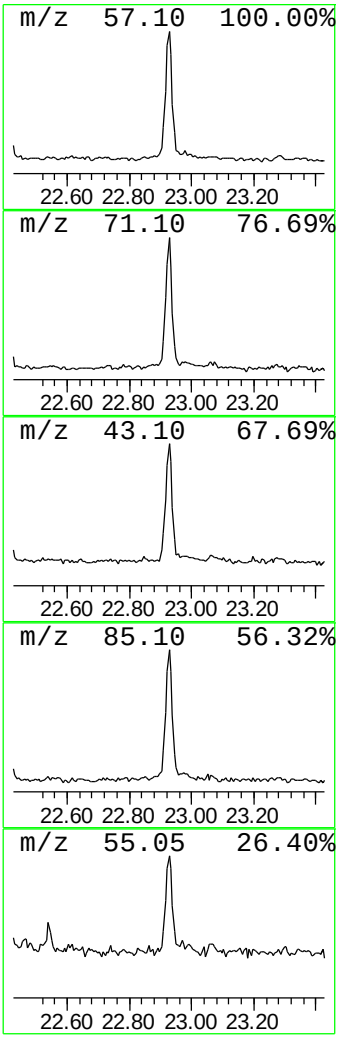
****

Peak Number 8 Pentadecane, 8-hexyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.93	2.11 ng	675272	Perylene-d12	23.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	93
2	Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
3	Eicosane	282	C20H42	000112-95-8	93
4	Pentacosane	352	C25H52	000629-99-2	91
5	Heneicosane	296	C21H44	000629-94-7	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM010919\
Data File : BM018475.D
Acq On : 09 Jan 2019 16:28
Operator : JU/SJ
Sample : K1088-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CPSB-05(10-15)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

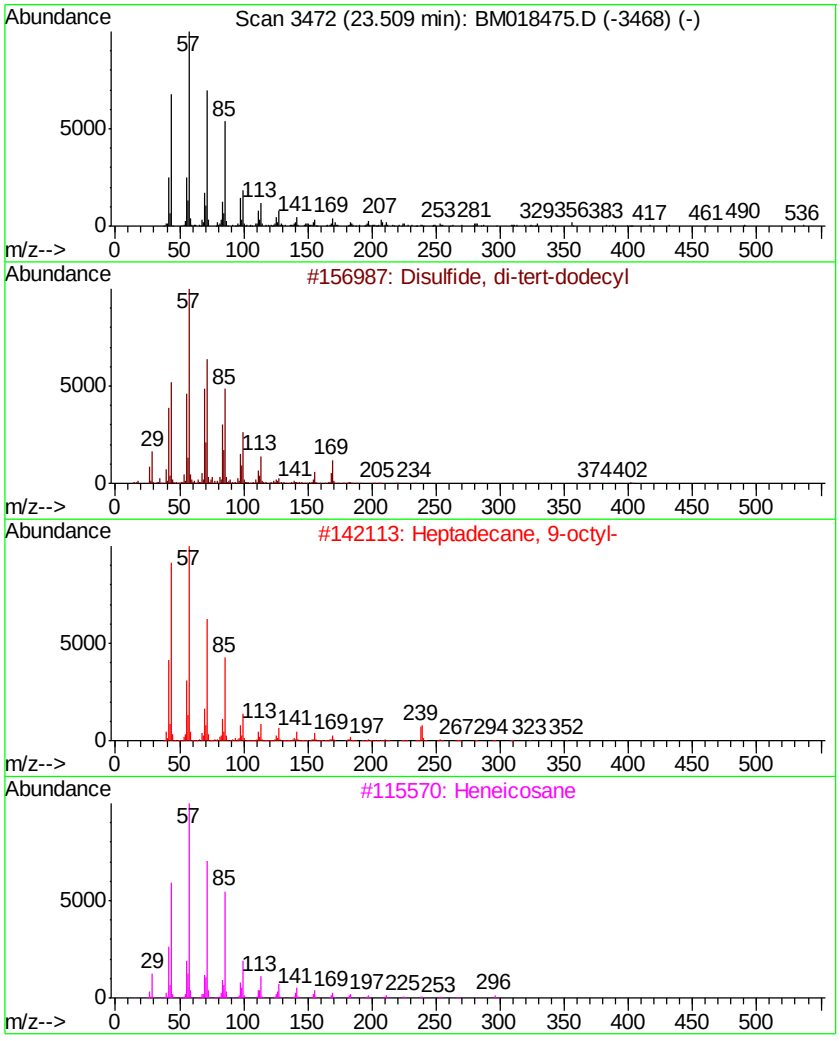
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

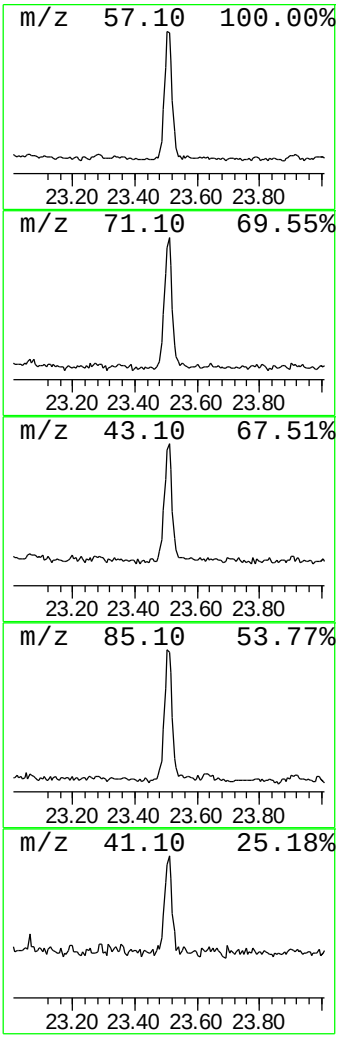
****

Peak Number 9 Disulfide, di-tert-dodecyl Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.51	2.31 ng	740633	Perylene-d12	23.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Disulfide, di-tert-dodecyl	402	C24H50S2	027458-90-8	93
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
3	Heneicosane	296	C21H44	000629-94-7	87
4	Tetracosane	338	C24H50	000646-31-1	87
5	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM010919\
Data File : BM018475.D
Acq On : 09 Jan 2019 16:28
Operator : JU/SJ
Sample : K1088-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CPSB-05(10-15)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.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...	4.90	3.9	ng	555893	1	7.76	2865900	20.0
unknown7.30	7.30	104.5	ng	14968000	1	7.76	2865900	20.0
n-Hexadecanoic acid	18.05	18.4	ng	5542410	4	17.16	6014310	20.0
6-Octadecenoic ac...	19.22	2.2	ng	650948	4	17.16	6014310	20.0
Octadecanoic acid	19.33	18.4	ng	6518670	5	21.35	7084000	20.0
Cycloeicosane	21.06	4.3	ng	1540300	5	21.35	7084000	20.0
Pentadecane, 8-he...	22.93	2.1	ng	675272	6	23.64	6405230	20.0
Disulfide, di-ter...	23.51	2.3	ng	740633	6	23.64	6405230	20.0