LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121918\
Data File : BM018309.D
Acq On : 19 Dec 2018 22:48
Operator : JU/SJ
Sample : J6378-22
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P001-SS002-0006-01

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	4.681	300	305	312	rVB	73710	97703	3.15%	0.299%
2	5.122	374	380	395	rBV	1950887	2819474	90.78%	8.632%
3	6.687	639	646	663	rBV	1847821	3056084	98.40%	9.357%
4	7.028	697	704	716	rBV	1997478	3105799	100.00%	9.509%
5	7.481	775	781	790	rBV	481648	755571	24.33%	2.313%
6	7.798	824	835	845	rBV	1468148	2333103	75.12%	7.143%
7	8.639	971	978	993	rBV	1009322	1797455	57.87%	5.503%
8	10.251	1245	1252	1264	rBV	501174	909540	29.29%	2.785%
9	12.745	1670	1676	1689	rBV	1895648	2886849	92.95%	8.839%
10	13.621	1819	1825	1838	rVB	113551	183180	5.90%	0.561%
11	14.145	1907	1914	1923	rBV2	654405	1020303	32.85%	3.124%
12	15.651	2164	2170	2183	rBV	1668578	2429214	78.22%	7.437%
13	16.327	2280	2285	2291	rBV8	19192	34682	1.12%	0.106%
14	16.821	2364	2369	2376	rBV4	29105	47908	1.54%	0.147%
15	16.904	2377	2383	2389	rVV2	720708	1094221	35.23%	3.350%
16	16.956	2389	2392	2396	rVV3	69135	95284	3.07%	0.292%
17	17.280	2443	2447	2452	rBV4	21216	37975	1.22%	0.116%
18	17.698	2513	2518	2523	rBV5	29810	50616	1.63%	0.155%
19	17.821	2533	2539	2554	rBV	558855	804476	25.90%	2.463%
20	18.115	2584	2589	2595	rBV10	16131	34693	1.12%	0.106%
21	18.986	2730	2737	2740	rBV	111499	194213	6.25%	0.595%
22	19.115	2754	2759	2771	rBV	212102	340458	10.96%	1.042%
23	19.350	2795	2799	2802	rVB	59126	72558	2.34%	0.222%
24	19.556	2829	2834	2842	rBV	2194883	2769457	89.17%	8.479%
25	19.856	2882	2885	2889	rVB5	27832	33476	1.08%	0.102%
26	20.850	3050	3054	3062	rVB	427838	535295	17.24%	1.639%
27	21.127	3095	3101	3105	rBV	1157309	1601234	51.56%	4.902%
28	21.709	3197	3200	3202	rBV3	124563	151645	4.88%	0.464%
29	22.156	3272	3276	3281	rVB3	249776	313675	10.10%	0.960%
30	22.638	3354	3358	3363	rBV2	347695	620114	19.97%	1.899%
31	22.686	3363	3366	3373	rVB3	355958	559819	18.02%	1.714%
32	23.285	3462	3468	3474	rBV	840495	1496718	48.19%	4.582%
33	23.774	3547	3551	3557	rVB	226218	379191	12.21%	1.161%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121918\
Data File : BM018309.D
Acq On : 19 Dec 2018 22:48
Operator : JU/SJ
Sample : J6378-22
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P001-SS002-0006-01

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

Sum of corrected areas: 32661983

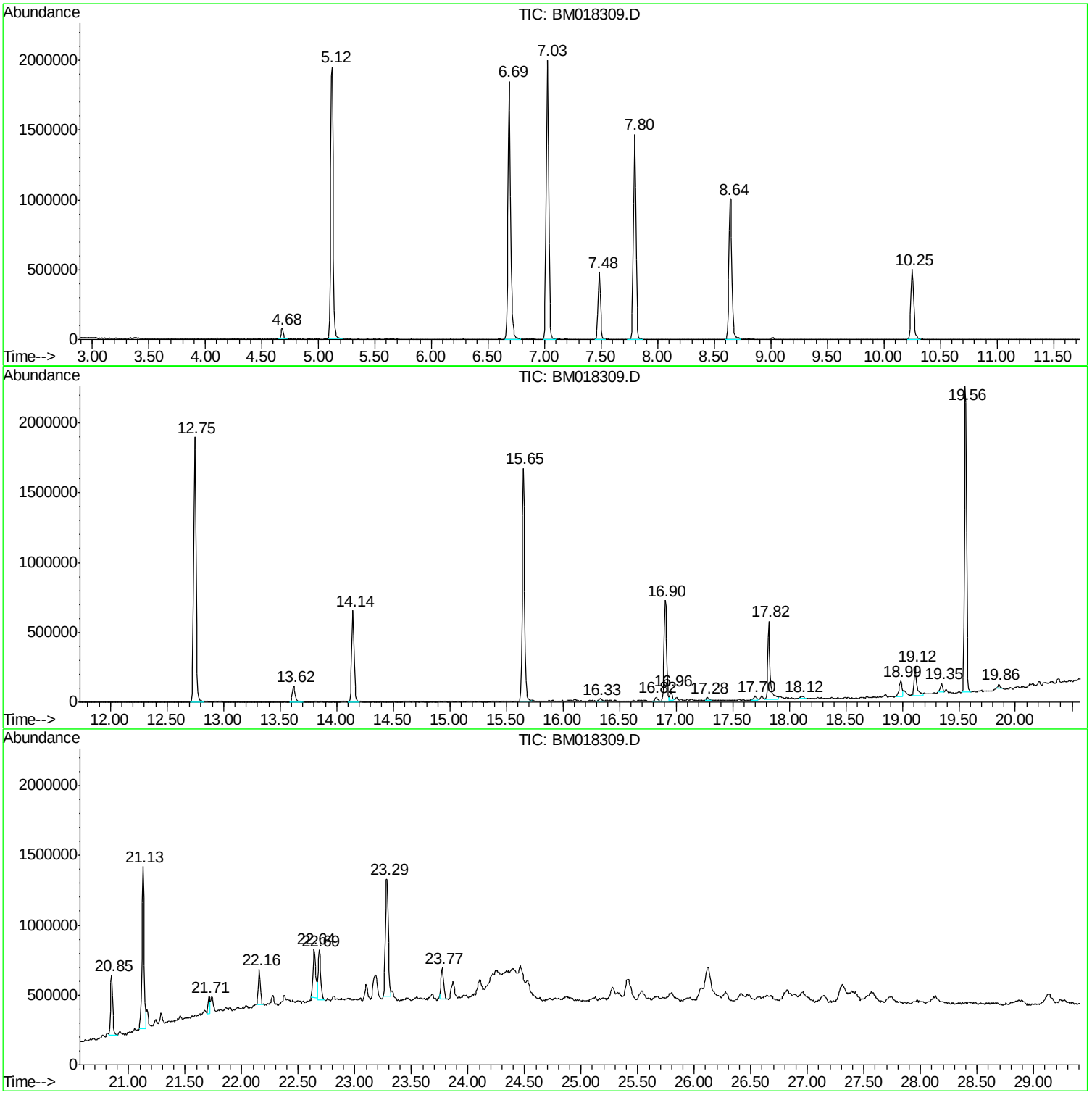
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121918\
Data File : BM018309.D
Acq On : 19 Dec 2018 22:48
Operator : JU/SJ
Sample : J6378-22
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P001-SS002-0006-01

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121918\
Data File : BM018309.D
Acq On : 19 Dec 2018 22:48
Operator : JU/SJ
Sample : J6378-22
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P001-SS002-0006-01

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

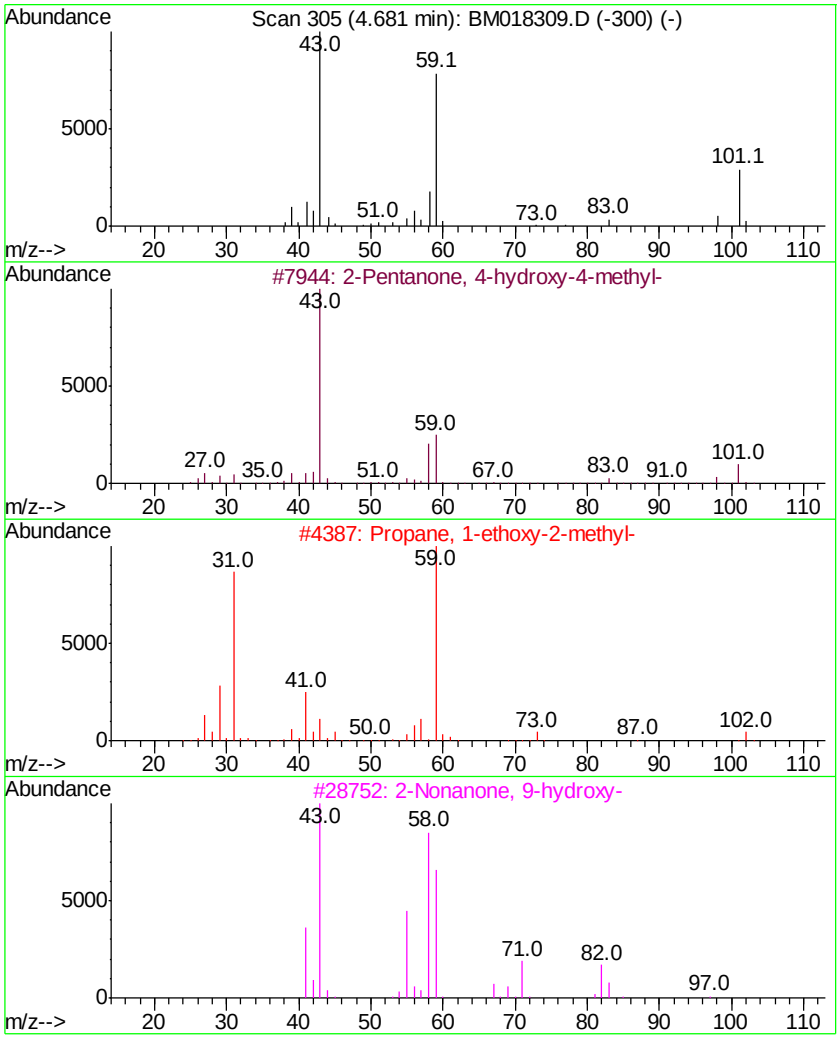
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

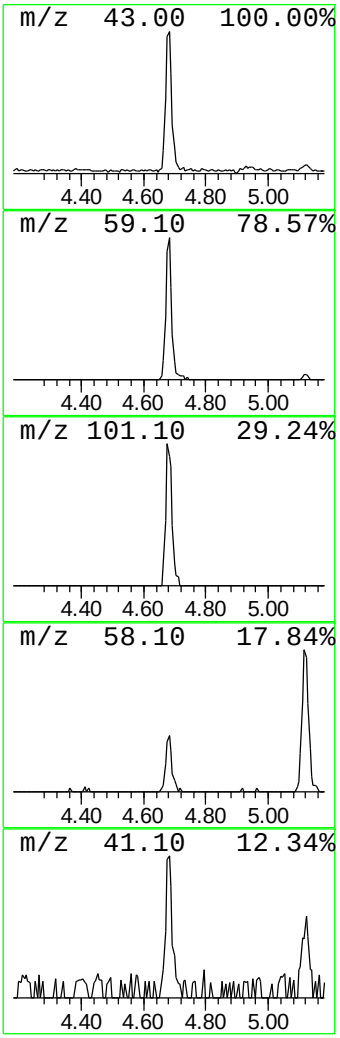
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.68	2.59 ng	97703	1,4-Dichlorobenzene-d4	7.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	37
3	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	36
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	35
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121918\
Data File : BM018309.D
Acq On : 19 Dec 2018 22:48
Operator : JU/SJ
Sample : J6378-22
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P001-SS002-0006-01

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

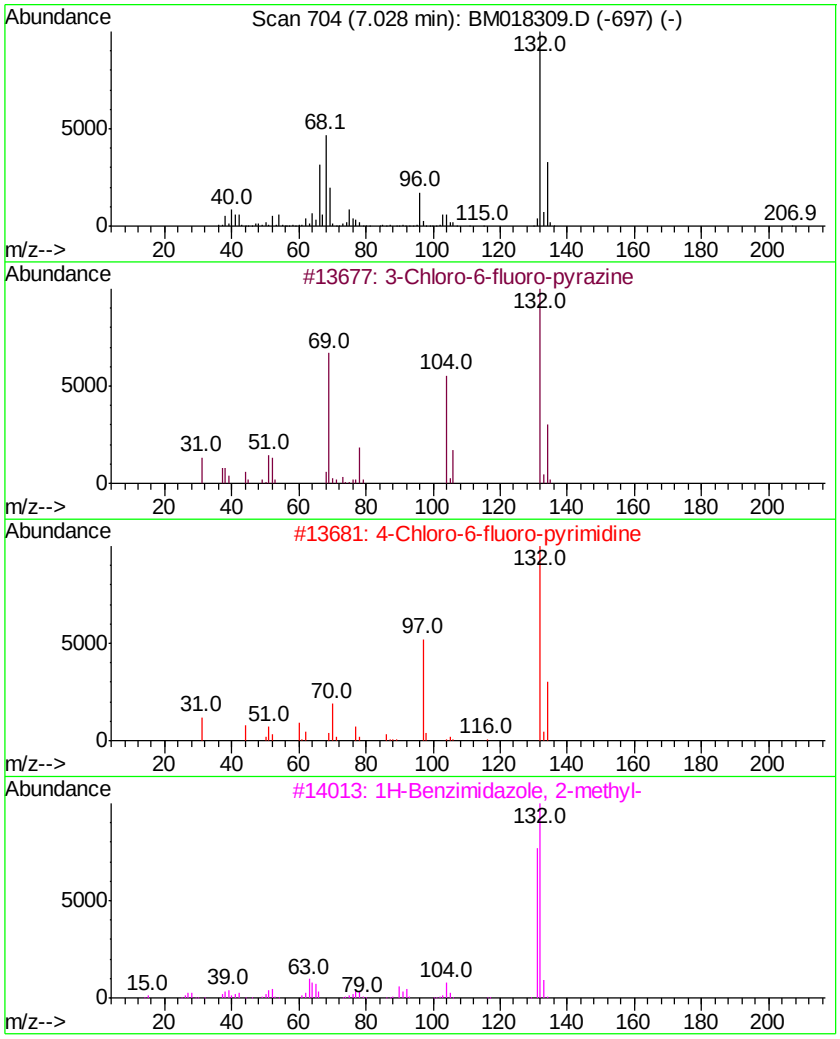
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

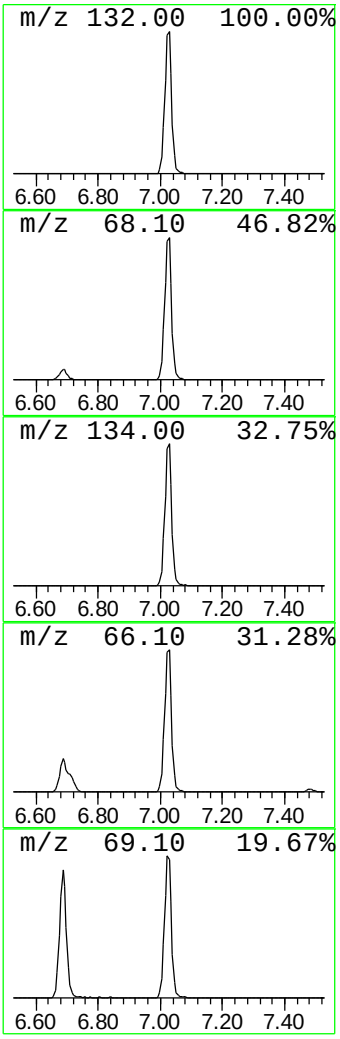
****

Peak Number 2 unknown7.03 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.03	82.21 ng	3105800	1,4-Dichlorobenzene-d4	7.48

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	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121918\
Data File : BM018309.D
Acq On : 19 Dec 2018 22:48
Operator : JU/SJ
Sample : J6378-22
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P001-SS002-0006-01

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

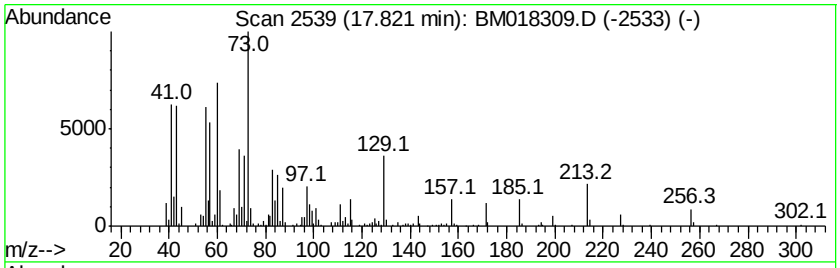
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

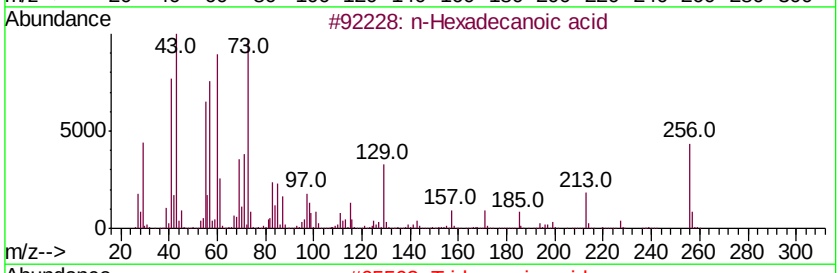
****

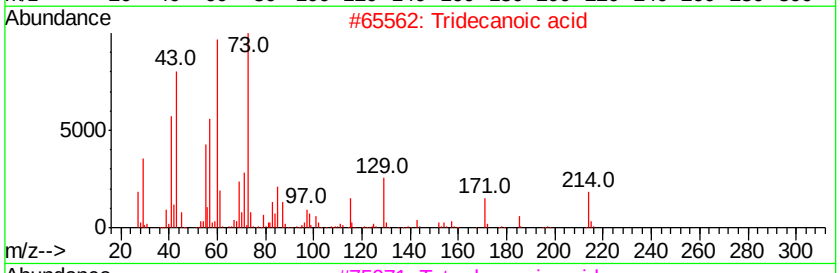
Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

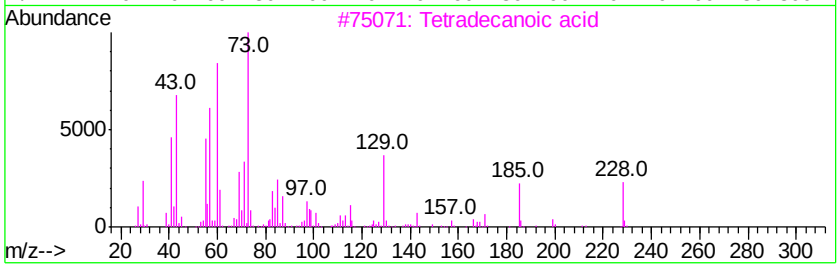
R.T.	EstConc	Area	Relative to ISTD	R.T.
17.82	14.70 ng	804476	Phenanthrene-d10	16.90

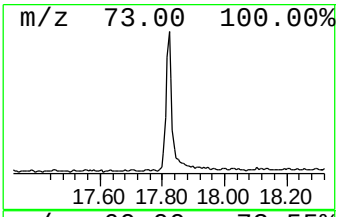
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	50

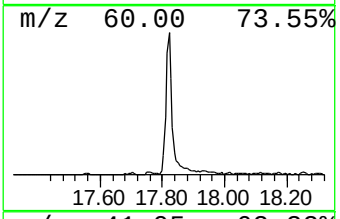


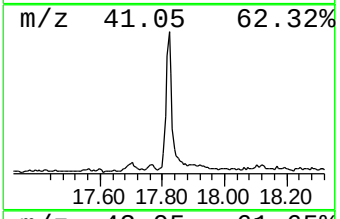


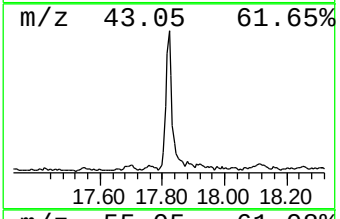


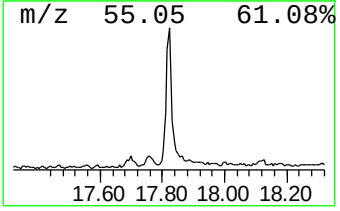












Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121918\
Data File : BM018309.D
Acq On : 19 Dec 2018 22:48
Operator : JU/SJ
Sample : J6378-22
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P001-SS002-0006-01

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

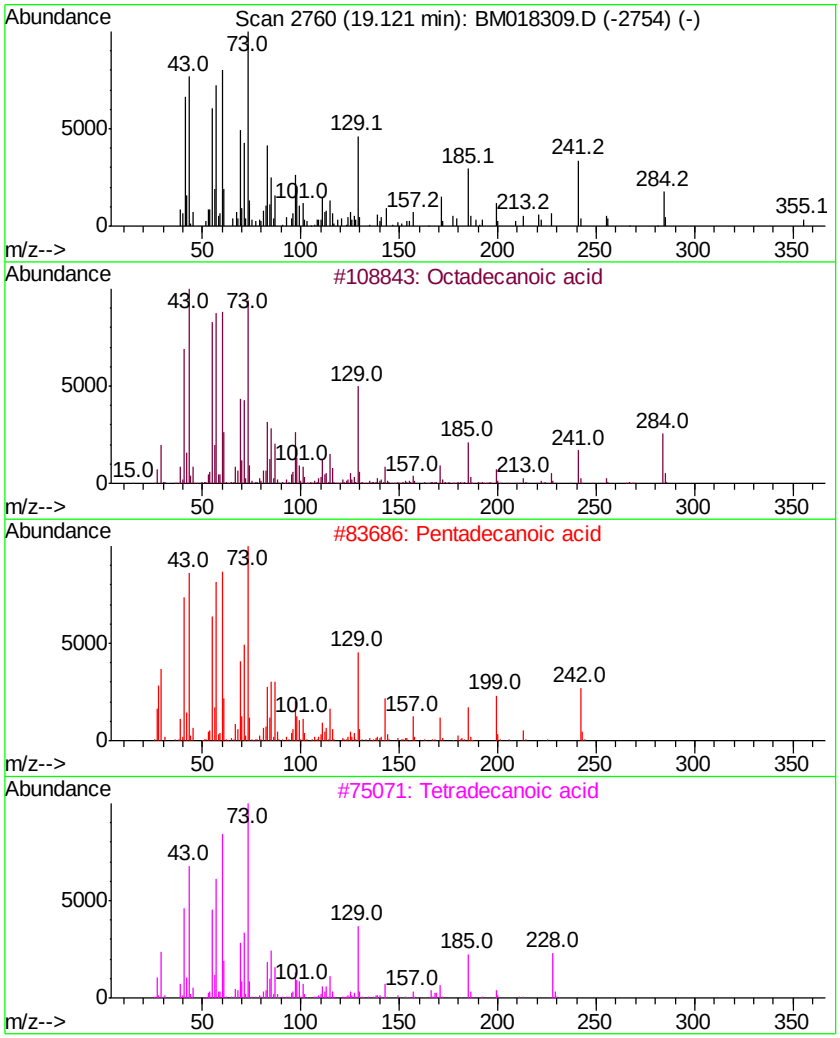
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

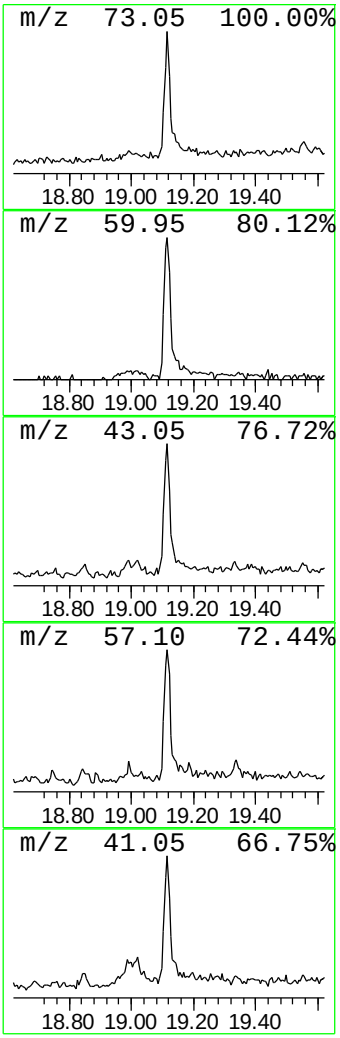
****

Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.12	4.25 ng	340458	Chrysene-d12	21.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	70
4	n-Decanoic acid	172	C10H20O2	000334-48-5	58
5	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	25





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Data File : BM018309.D
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Sample : J6378-22
Misc :
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Instrument : BNA_M
ClientSampleId : P001-SS002-0006-01

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

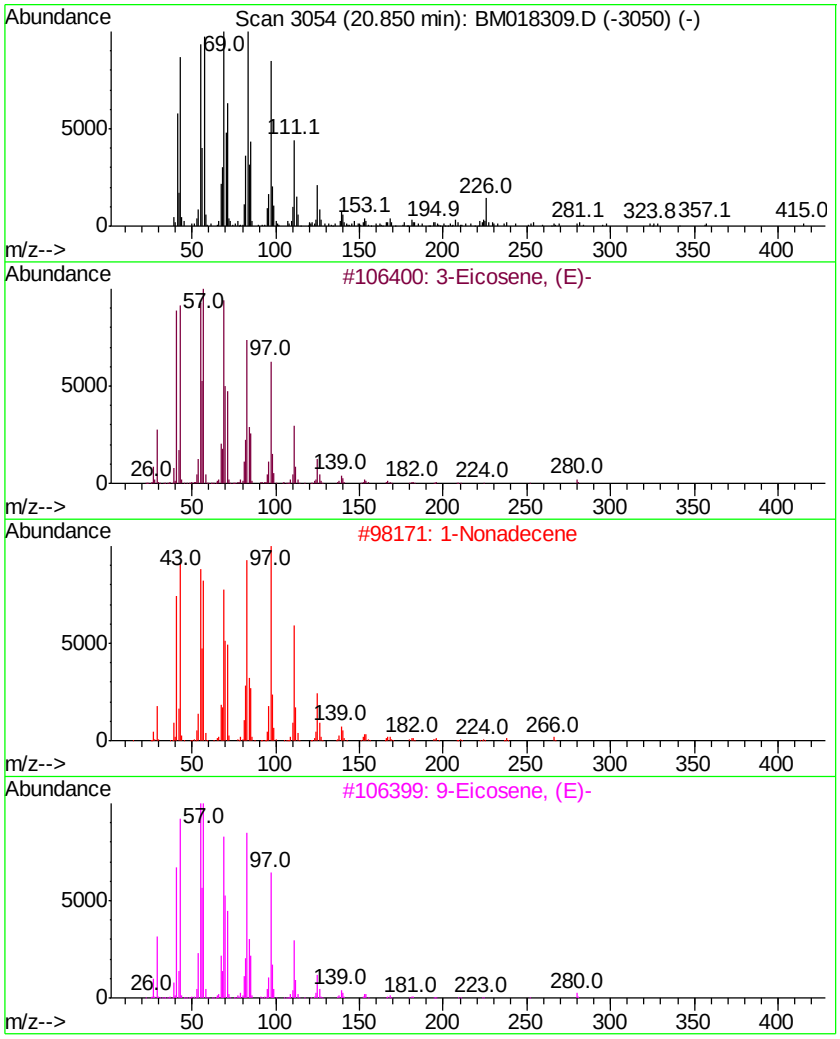
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

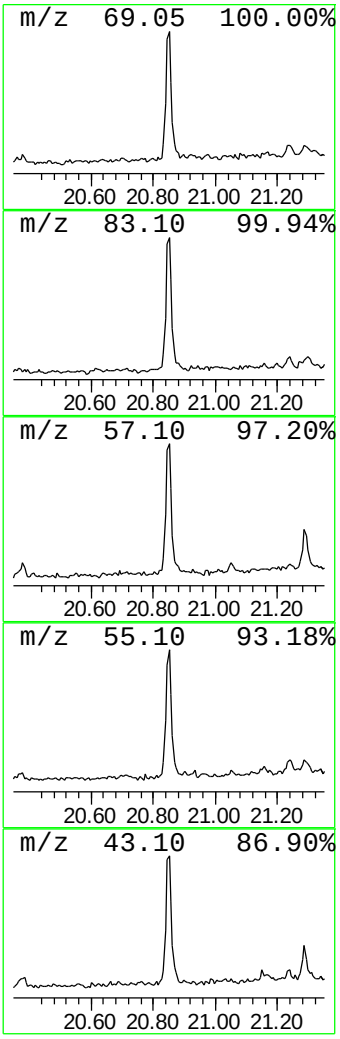
****

Peak Number 7 3-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.85	6.69 ng	535295	Chrysene-d12	21.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	99
2	1-Nonadecene	266	C19H38	018435-45-5	97
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	93
4	Cyclohexadecane	224	C16H32	000295-65-8	93
5	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	93





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Data File : BM018309.D
Acq On : 19 Dec 2018 22:48
Operator : JU/SJ
Sample : J6378-22
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P001-SS002-0006-01

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

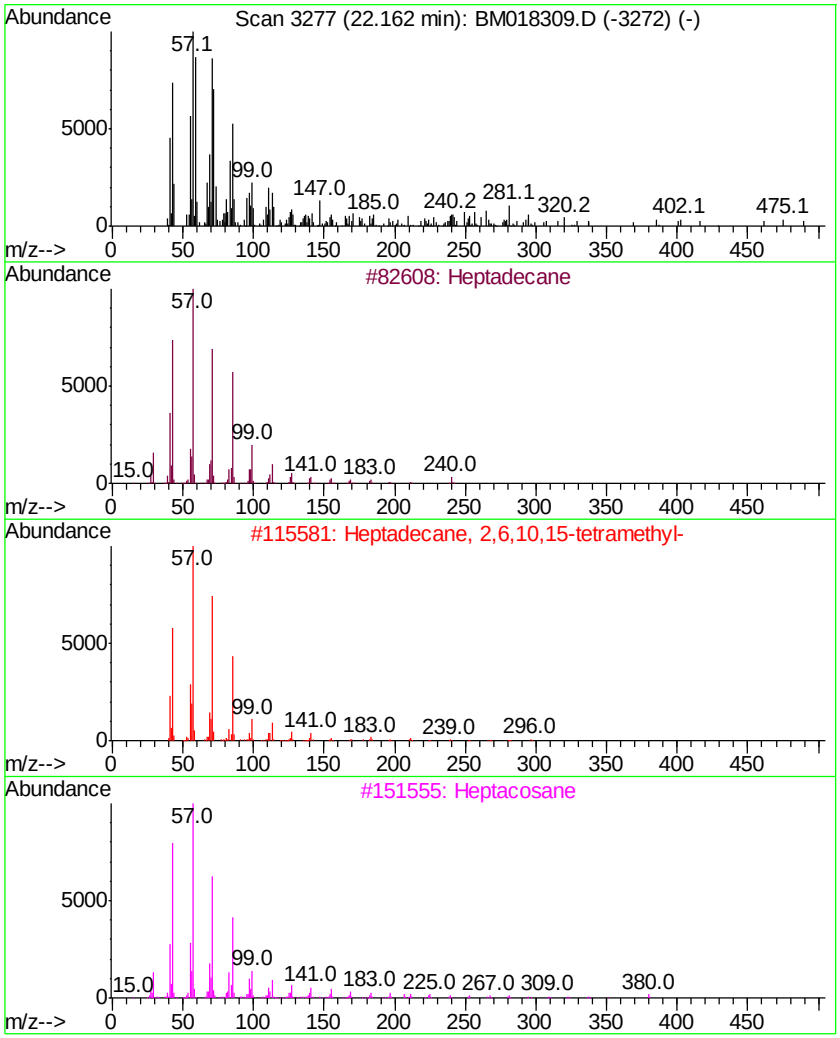
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

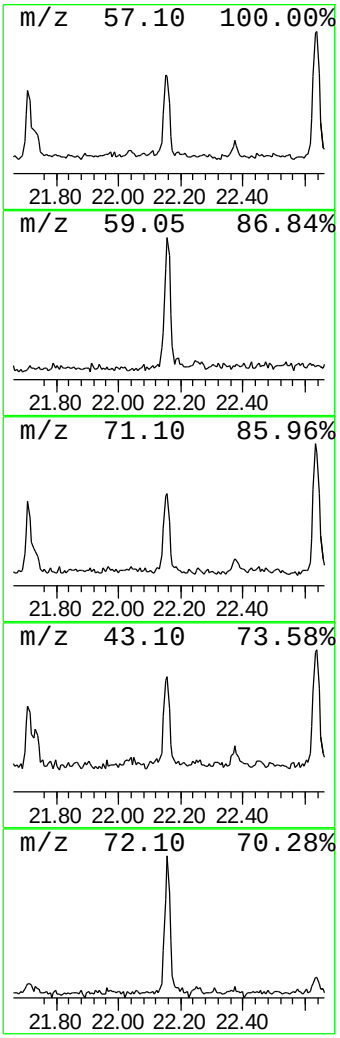
****

Peak Number 8 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.16	3.92 ng	313675	Chrysene-d12	21.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	78
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	60
3	Heptacosane	380	C27H56	000593-49-7	53
4	Tetratriacontane	479	C34H70	014167-59-0	49
5	Hexadecane	226	C16H34	000544-76-3	49





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121918\
Data File : BM018309.D
Acq On : 19 Dec 2018 22:48
Operator : JU/SJ
Sample : J6378-22
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P001-SS002-0006-01

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

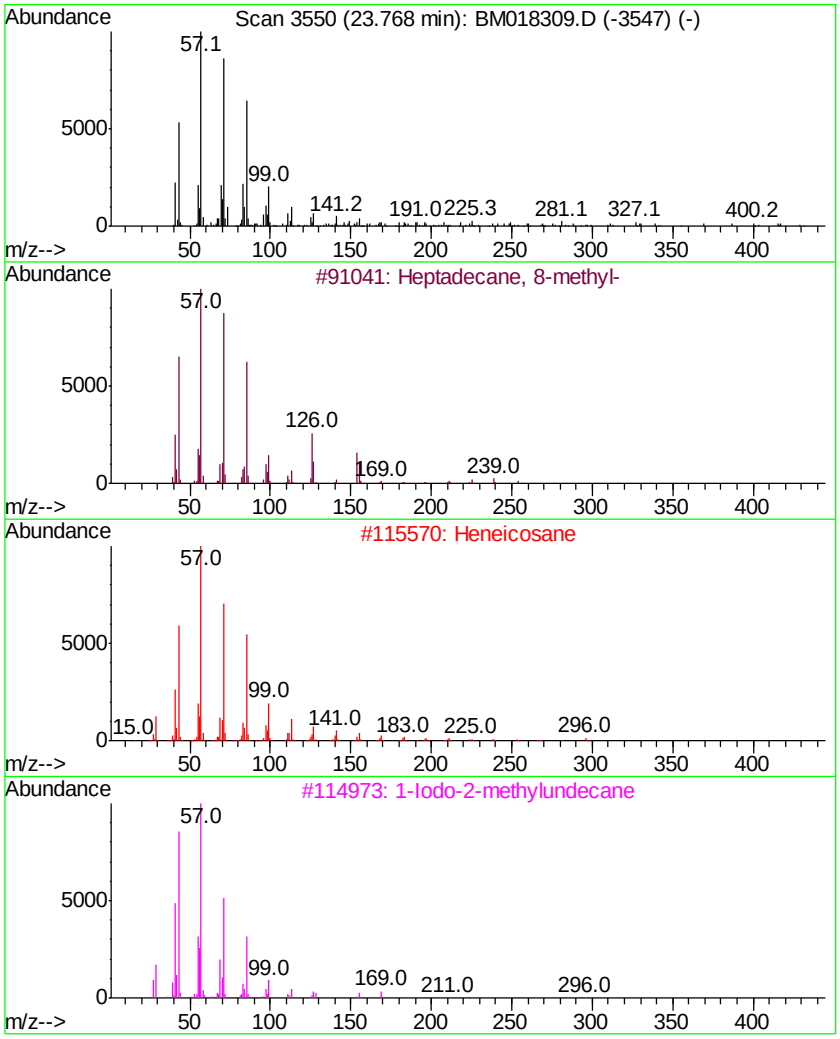
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

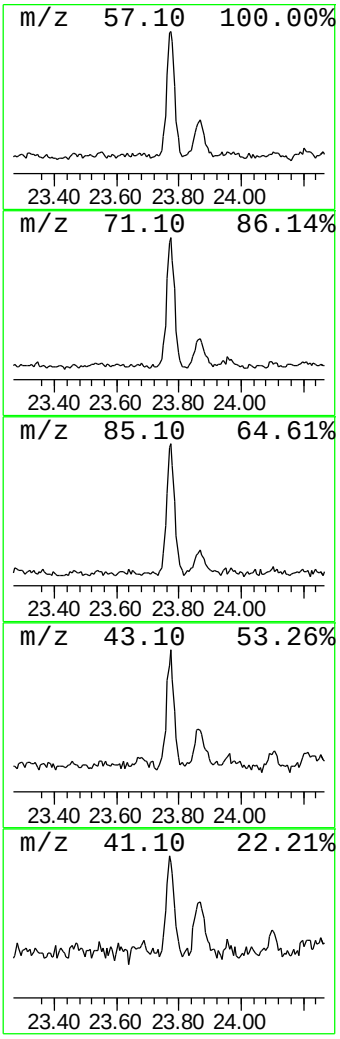
****

Peak Number 9 Heptadecane, 8-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.77	5.07 ng	379191	Perylene-d12	23.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 8-methyl-	254	C18H38	013287-23-5	91
2	Heneicosane	296	C21H44	000629-94-7	90
3	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	90
4	Dodecane, 2-methyl-	184	C13H28	001560-97-0	87
5	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM121918\
Data File : BM018309.D
Acq On : 19 Dec 2018 22:48
Operator : JU/SJ
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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	2.6	ng	97703	1	7.48	755571	20.0
unknown7.03	7.03	82.2	ng	3105800	1	7.48	755571	20.0
n-Hexadecanoic acid	17.82	14.7	ng	804476	4	16.90	1094220	20.0
Octadecanoic acid	19.12	4.3	ng	340458	5	21.13	1601230	20.0
3-Eicosene, (E)-	20.85	6.7	ng	535295	5	21.13	1601230	20.0
Heptadecane	22.16	3.9	ng	313675	5	21.13	1601230	20.0
Heptadecane, 8-me...	23.77	5.1	ng	379191	6	23.29	1496720	20.0