LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM021318\
Data File : BM014220.D
Acq On : 13 Feb 2018 14:33
Operator : SJ/JU
Sample : J1518-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-6

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:\HPCHEM1\BNA_M\METHODS\8270-BM020718.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	5.163	364	370	386	rBV	411479	713681	14.13%	2.817%
2	6.734	631	637	652	rBV2	250851	468128	9.27%	1.848%
3	7.075	688	695	709	rBV	938522	1519316	30.08%	5.997%
4	7.540	768	774	784	rBV	353282	580010	11.48%	2.289%
5	7.851	819	827	838	rBV	926391	1523495	30.16%	6.014%
6	8.698	964	971	985	rBV	663273	1266414	25.07%	4.999%
7	10.310	1238	1245	1260	rBV	388587	760104	15.05%	3.000%
8	12.804	1662	1669	1685	rBV	1946818	2967869	58.75%	11.715%
9	13.674	1808	1817	1822	rBV	81875	147316	2.92%	0.581%
10	14.098	1884	1889	1896	rBV2	79730	112646	2.23%	0.445%
11	14.192	1898	1905	1916	rVV2	674103	1092356	21.62%	4.312%
12	15.057	2045	2052	2057	rVB3	91708	152817	3.03%	0.603%
13	15.698	2153	2161	2178	rBV	1579979	2468500	48.87%	9.744%
14	15.921	2195	2199	2207	rBV3	48862	84622	1.68%	0.334%
15	16.951	2368	2374	2386	rBV	920630	1407502	27.86%	5.556%
16	17.862	2523	2529	2538	rBV2	303585	476214	9.43%	1.880%
17	19.151	2741	2748	2759	rBV2	129602	231846	4.59%	0.915%
18	19.598	2818	2824	2830	rBV	4157724	5051621	100.00%	19.940%
19	20.880	3037	3042	3051	rBV	550483	845041	16.73%	3.336%
20	21.162	3084	3090	3102	rBV	1262117	1771829	35.07%	6.994%
21	23.333	3453	3459	3471	rVB	798681	1538578	30.46%	6.073%
22	23.909	3554	3557	3564	rVB7	84097	154066	3.05%	0.608%

Sum of corrected areas: 25333971

LSC Report - Integrated Chromatogram

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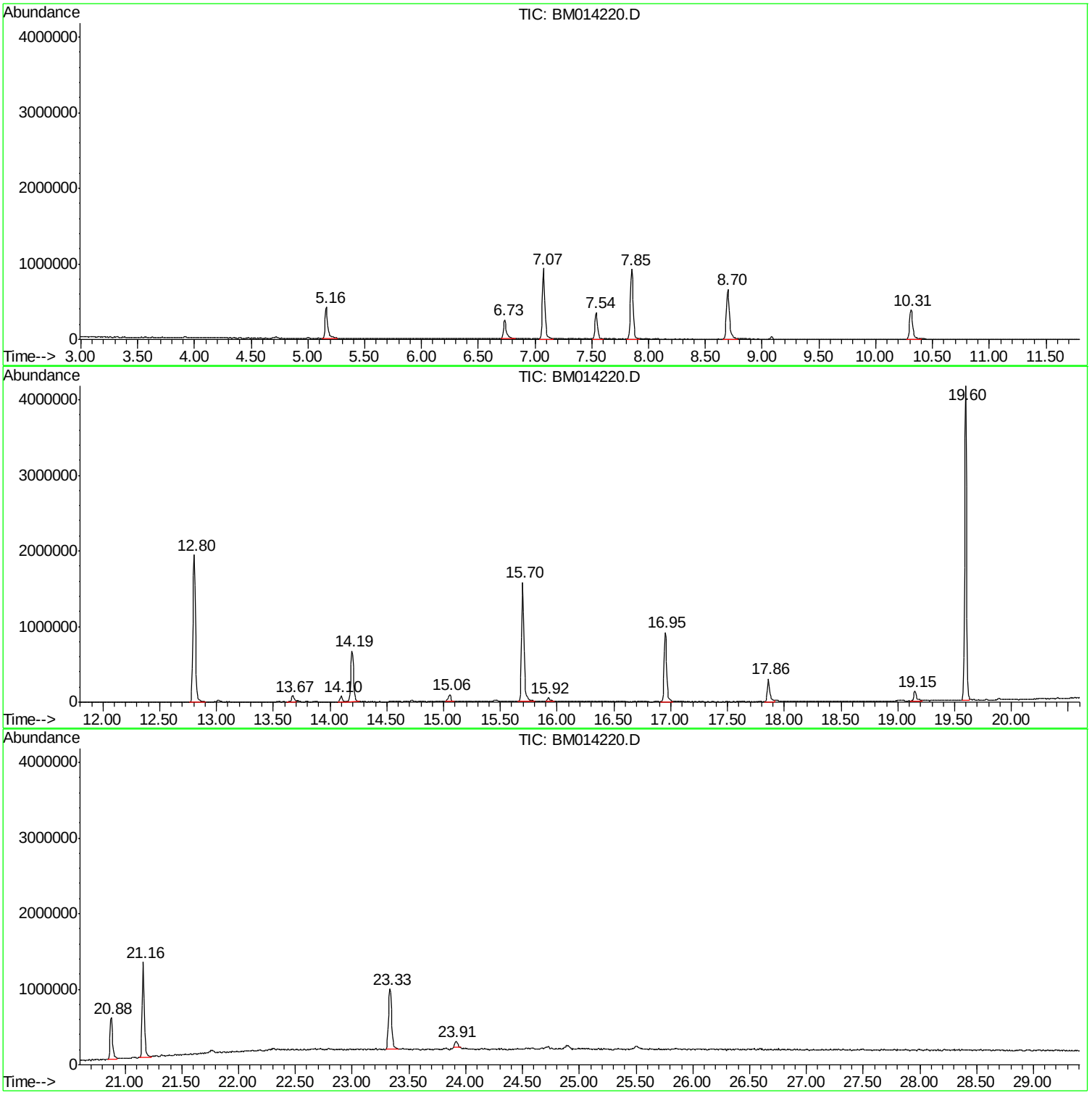
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-6

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM020718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA M\DATA\BM021318\
Data File : BM014220.D
Acq On : 13 Feb 2018 14:33
Operator : SJ/JU
Sample : J1518-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
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Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM020718.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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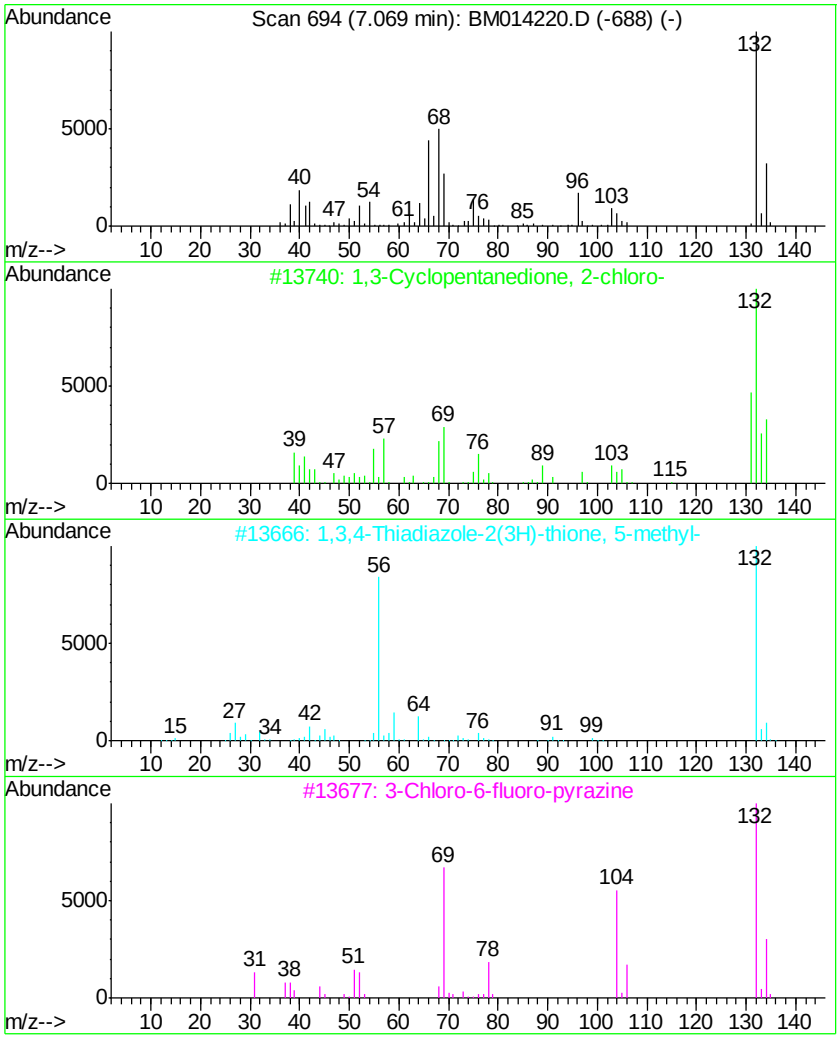
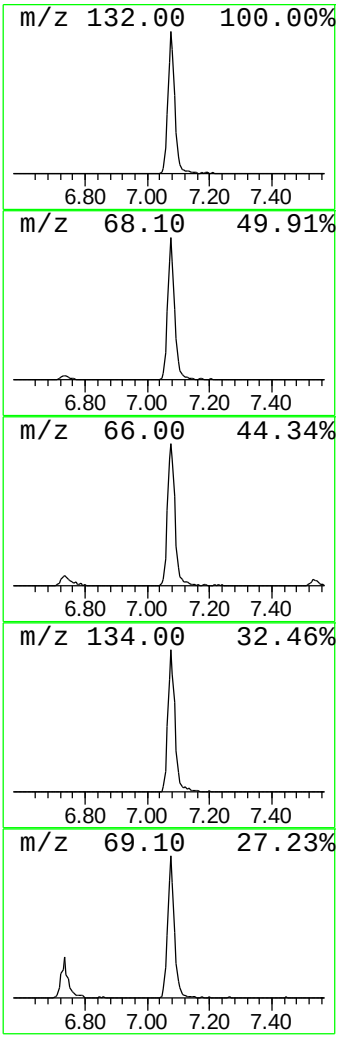
Peak Number 1 unknown7.07 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.07	52.39 ng	1519320	1,4-Dichlorobenzene-d4	7.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	27
2	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
3	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
5	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14





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Acq On : 13 Feb 2018 14:33
Operator : SJ/JU
Sample : J1518-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-6

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM020718.M
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TIC Library : C:\DATABASE\NIST02.L
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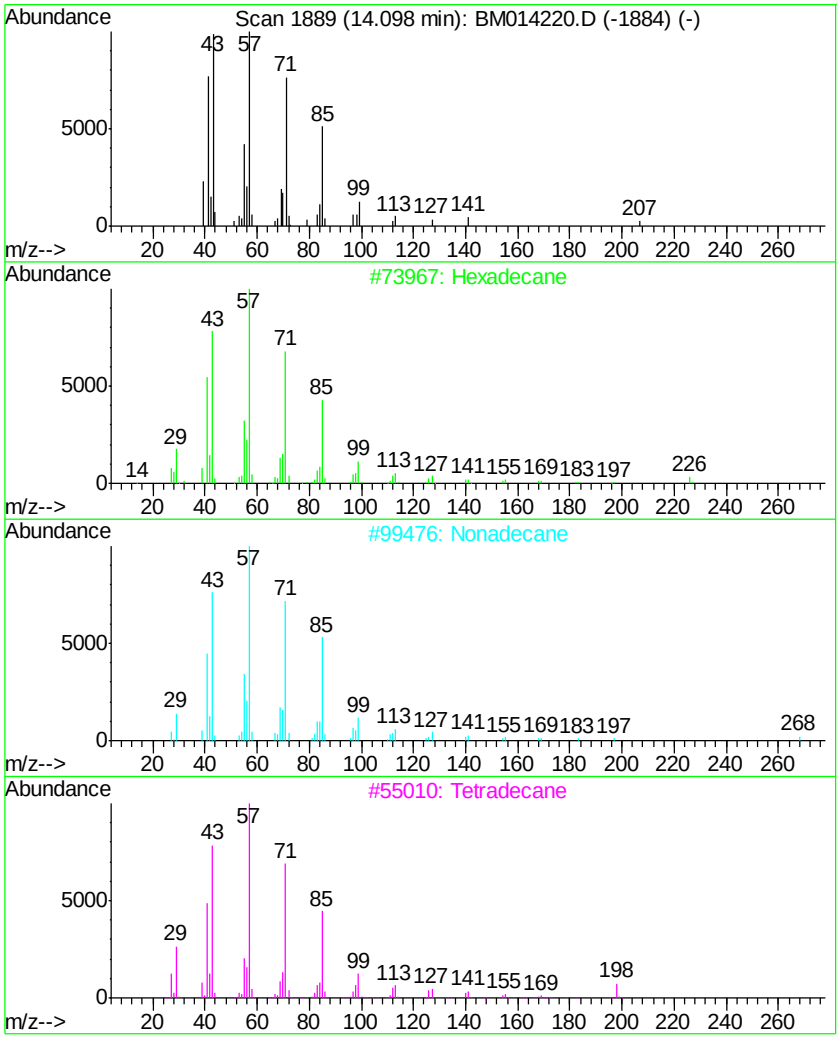
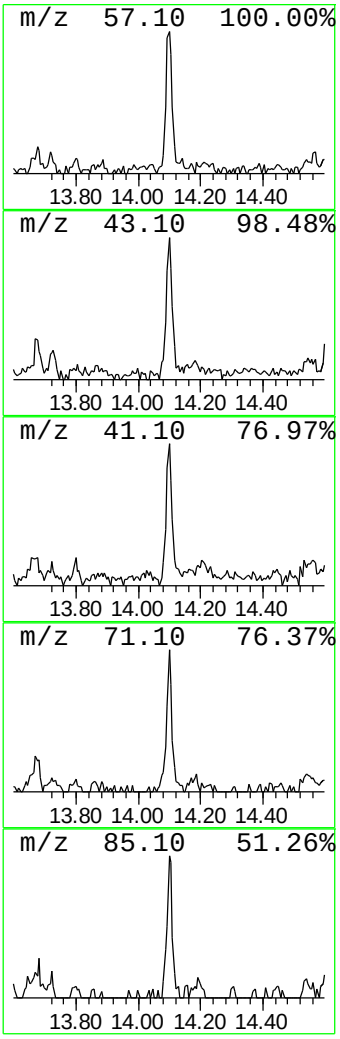
Peak Number 3 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.10	2.06 ng	112646	Acenaphthene-d10	14.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Nonadecane	268	C19H40	000629-92-5	91
3	Tetradecane	198	C14H30	000629-59-4	90
4	Tridecane, 7-propyl-	226	C16H34	055045-09-5	86
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	80





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM021318\
Data File : BM014220.D
Acq On : 13 Feb 2018 14:33
Operator : SJ/JU
Sample : J1518-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-6

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM020718.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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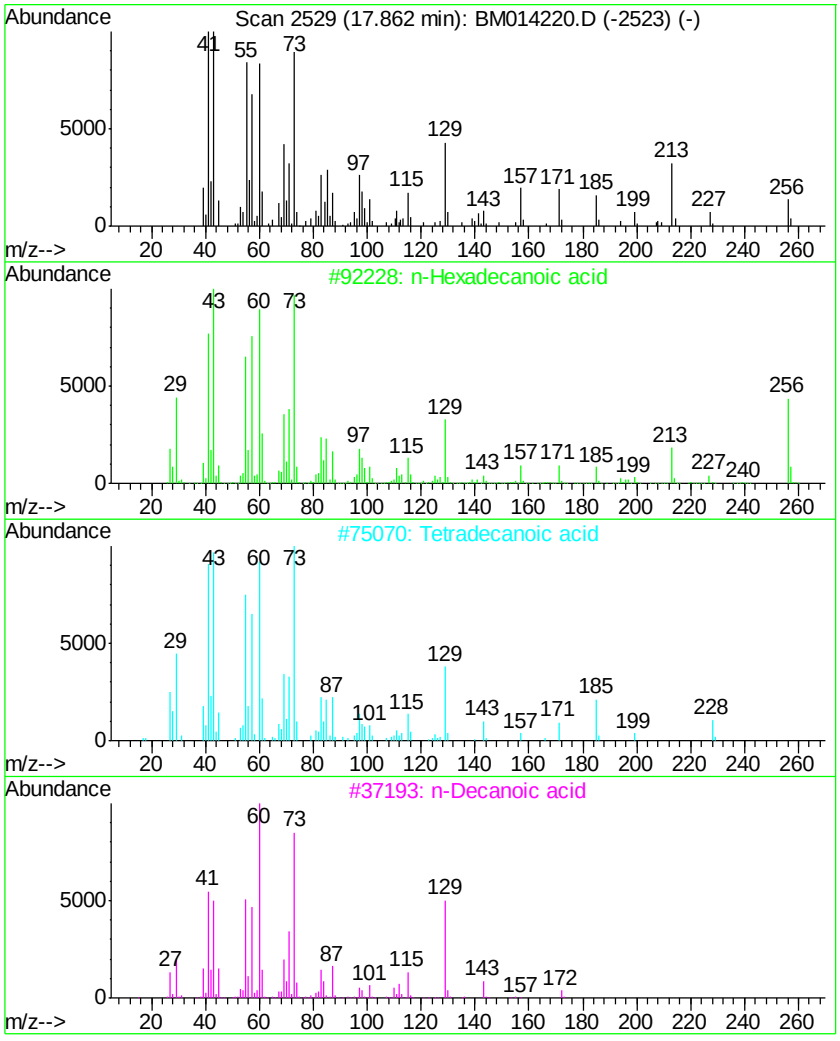
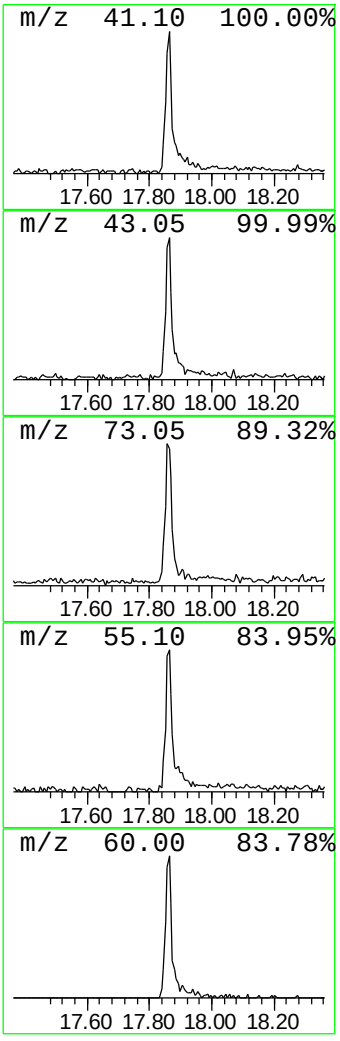
Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.86	6.77 ng	476214	Phenanthrene-d10	16.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	62
3	n-Decanoic acid	172	C10H20O2	000334-48-5	60
4	Dodecanoic acid	200	C12H24O2	000143-07-7	58
5	Tridecanoic acid	214	C13H26O2	000638-53-9	53





Library Search Compound Report

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Data File : BM014220.D
Acq On : 13 Feb 2018 14:33
Operator : SJ/JU
Sample : J1518-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-6

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM020718.M
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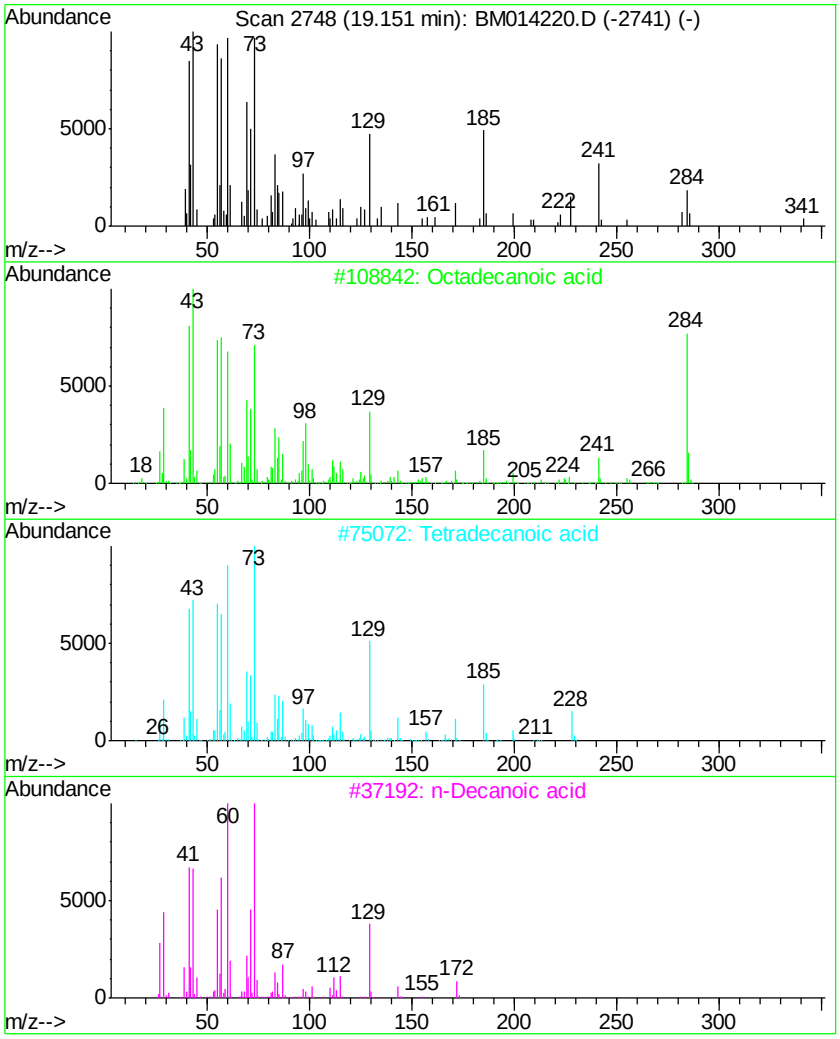
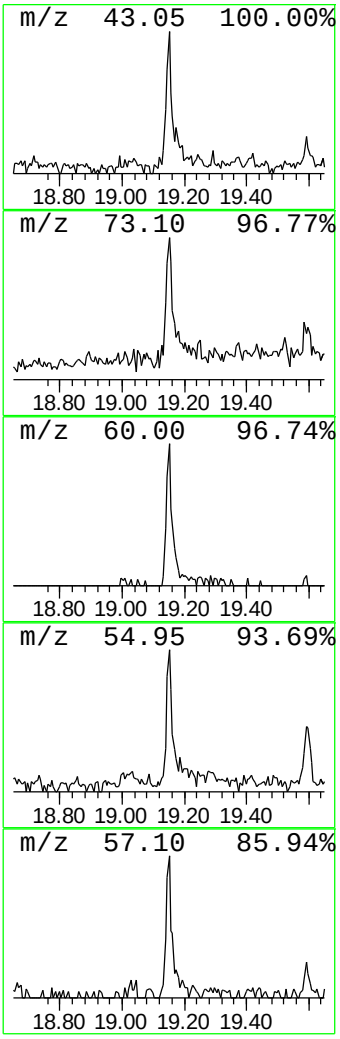
Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.15	2.62 ng	231846	Chrysene-d12	21.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	91
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
3	n-Decanoic acid	172	C10H20O2	000334-48-5	47
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	43
5	Tridecanoic acid	214	C13H26O2	000638-53-9	43





Data Path : Z:\HPCHEM1\BNA M\DATA\BM021318\
Data File : BM014220.D
Acq On : 13 Feb 2018 14:33
Operator : SJ/JU
Sample : J1518-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-6

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM020718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

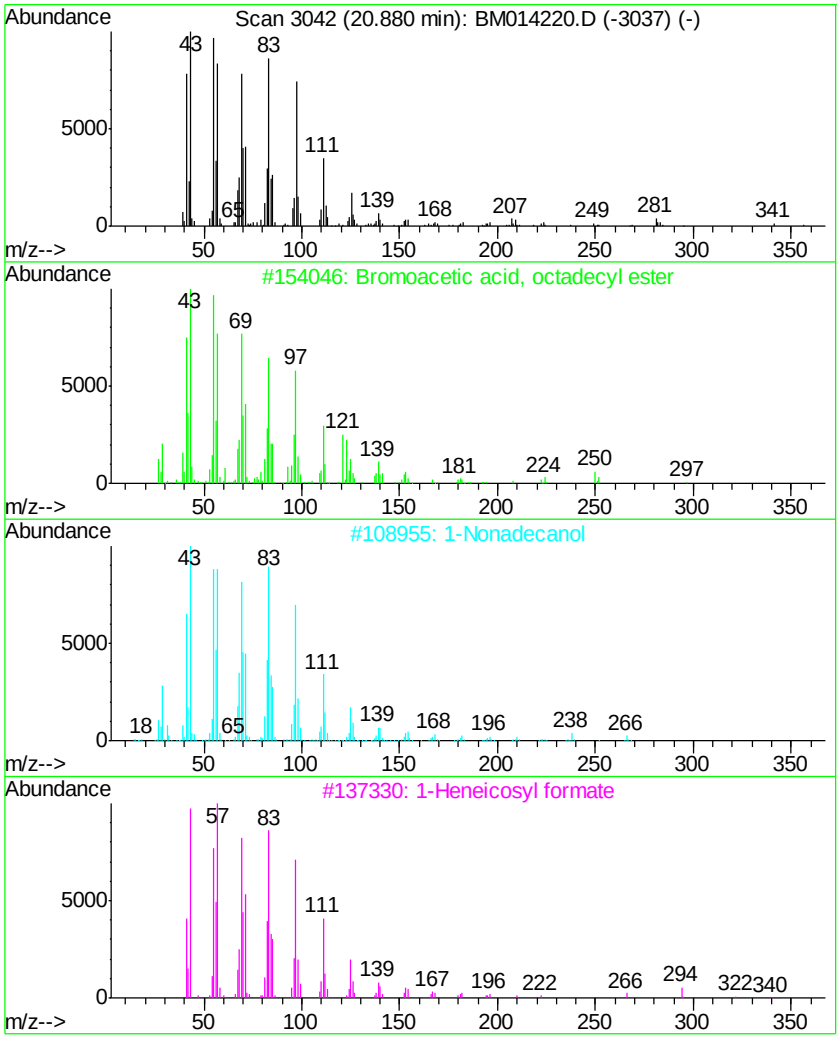
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

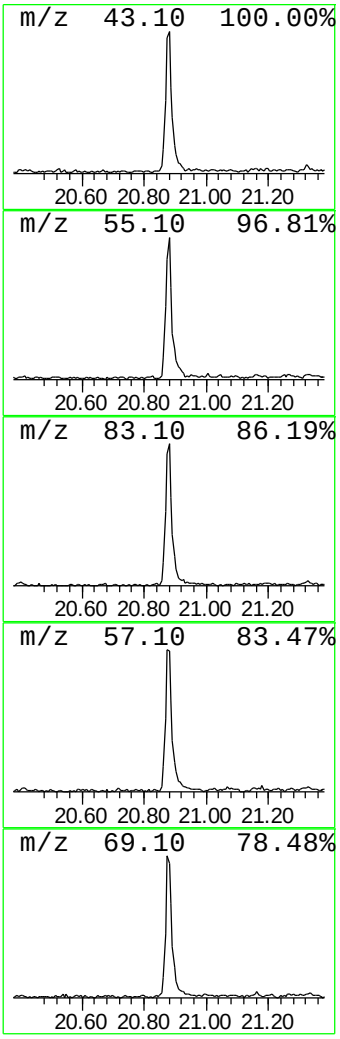
****

Peak Number 7 Bromoacetic acid, octadecyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.88	9.54 ng	845041	Chrysene-d12	21.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
2	1-Nonadecanol	284	C19H40O	001454-84-8	87
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	87
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	87
5	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	87





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Instrument : BNA_M
ClientSampleId : MW-6

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TIC Library : C:\DATABASE\NIST02.L
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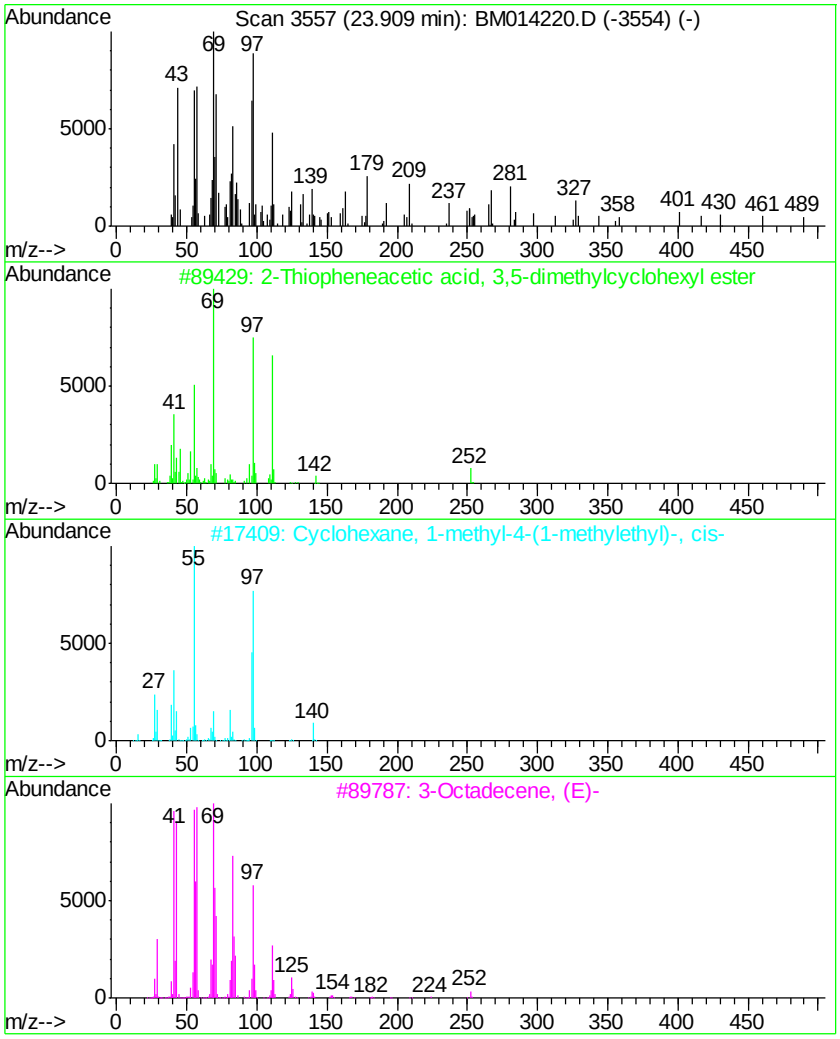
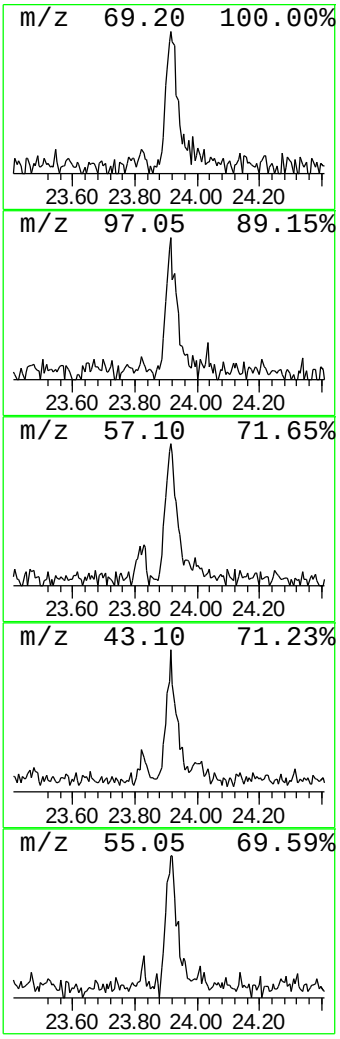
Peak Number 8 unknown23.91 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.91	2.00 ng	154066	Perylene-d12	23.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Thiopheneacetic acid, 3,5-dime...	252	C14H20O2S	1000278-92-2	46
2	Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	006069-98-3	35
3	3-Octadecene, (E)-	252	C18H36	007206-19-1	35
4	Cyclooctanemethanol	142	C9H18O	003637-63-6	35
5	Cyclohexane, 1-(cyclohexylmethyl...	194	C14H26	054823-95-9	35





Tentatively Identified Compound (LSC) summary

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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
unknown7.07	7.07	52.4	ng	1519320	1	7.54	580010	20.0
Hexadecane	14.10	2.1	ng	112646	3	14.19	1092360	20.0
n-Hexadecanoic acid	17.86	6.8	ng	476214	4	16.95	1407500	20.0
Octadecanoic acid	19.15	2.6	ng	231846	5	21.16	1771830	20.0
Bromoacetic acid,...	20.88	9.5	ng	845041	5	21.16	1771830	20.0
unknown23.91	23.91	2.0	ng	154066	6	23.33	1538580	20.0