LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080818\
Data File : BM016245.D
Acq On : 08 Aug 2018 12:10
Operator : SJ/JU
Sample : J4327-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : FK-BPM-02-007-ABCD

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-BM072318.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	5.187	318	323	336	rVB	117898	174045	9.02%	1.321%
2	5.663	398	404	422	rBV	784003	1183205	61.33%	8.977%
3	7.304	676	683	698	rBV	730892	1218124	63.14%	9.242%
4	7.663	738	744	758	rBV	861950	1355699	70.27%	10.286%
5	8.134	819	824	833	rBB	186907	299172	15.51%	2.270%
6	8.457	872	879	889	rBV	626038	1004288	52.05%	7.620%
7	9.322	1019	1026	1043	rBV	452632	761677	39.48%	5.779%
8	10.951	1296	1303	1314	rBV	206333	345812	17.92%	2.624%
9	13.392	1711	1718	1731	rBV	1017898	1449285	75.12%	10.996%
10	14.221	1855	1859	1866	rBV	69849	97957	5.08%	0.743%
11	14.768	1947	1952	1960	rBB2	249503	378274	19.61%	2.870%
12	16.257	2199	2205	2218	rBV	856650	1163237	60.29%	8.826%
13	17.503	2412	2417	2429	rVB	294934	418482	21.69%	3.175%
14	18.356	2557	2562	2571	rBV	136578	193620	10.04%	1.469%
15	19.615	2772	2776	2788	rBV	56426	80952	4.20%	0.614%
16	20.086	2850	2856	2861	rBV	1661532	1929302	100.00%	14.638%
17	21.303	3059	3063	3073	rBV	91249	161114	8.35%	1.222%
18	21.633	3115	3119	3125	rBV	376618	472008	24.47%	3.581%
19	23.974	3511	3517	3527	rVB2	257297	493812	25.60%	3.747%

Sum of corrected areas: 13180065

LSC Report - Integrated Chromatogram

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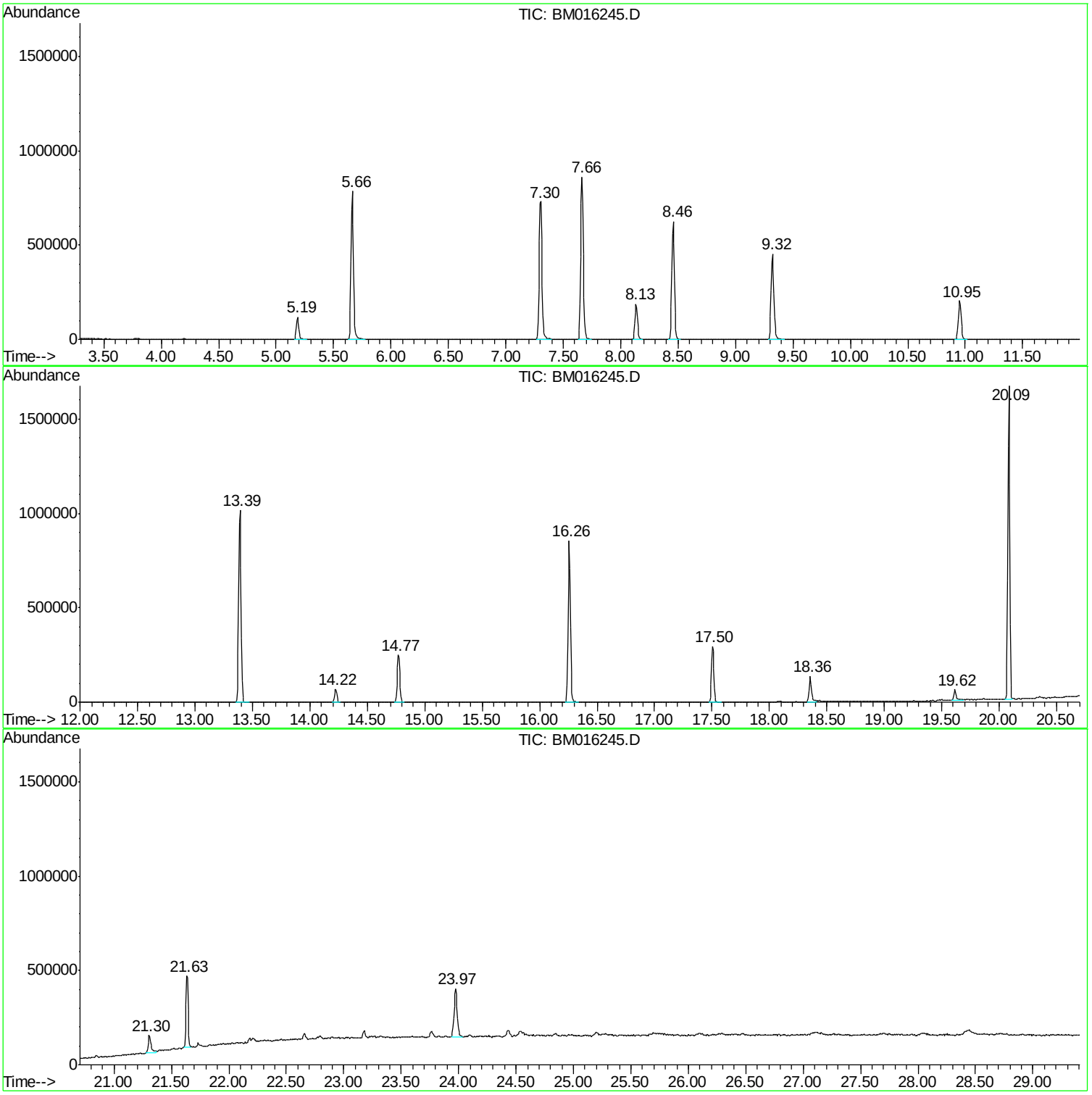
Sample : J4327-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FK-BPM-02-007-ABCD

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.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

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Data File : BM016245.D
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Instrument : BNA_M
ClientSampleId : FK-BPM-02-007-ABCD

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

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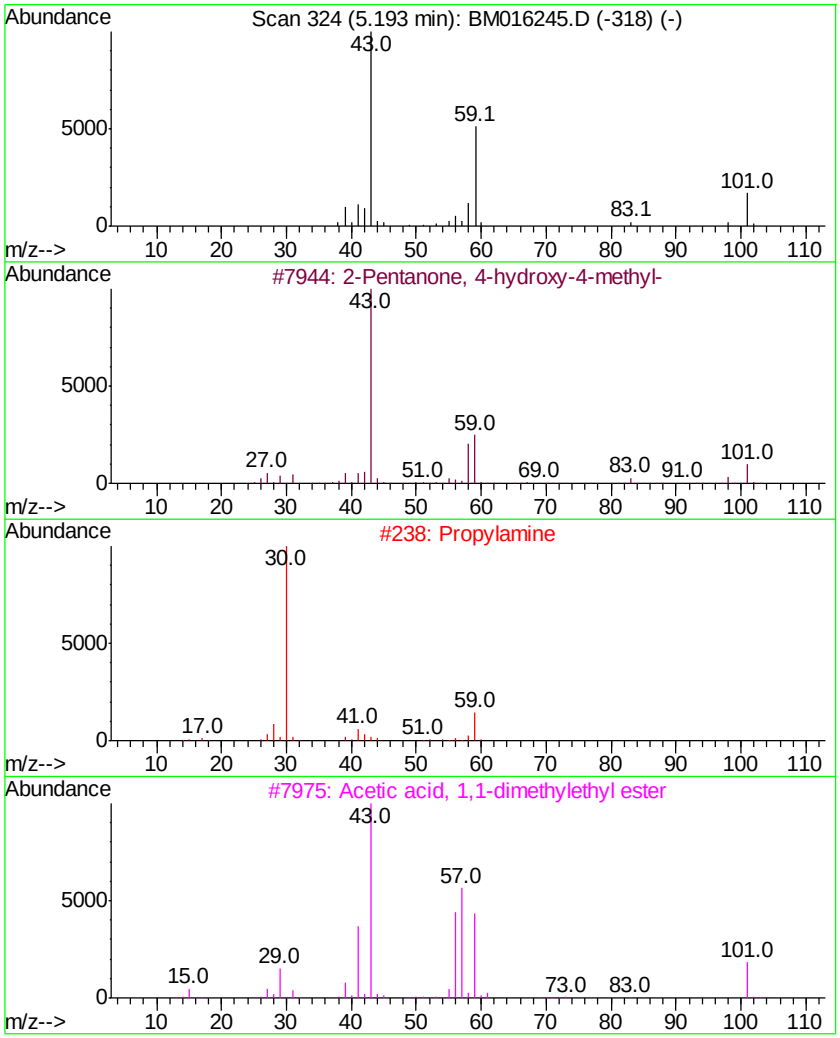
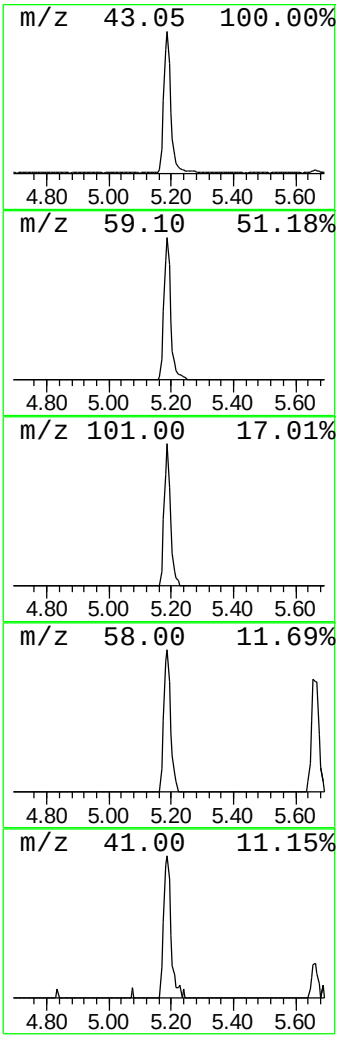
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	11.64 ng	174045	1,4-Dichlorobenzene-d4	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Propylamine	59	C3H9N	000107-10-8	42
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	36
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
5	Butane, 1-(1-methylethoxy)-	116	C7H16O	001860-27-1	25





Library Search Compound Report

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Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : FK-BPM-02-007-ABCD

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.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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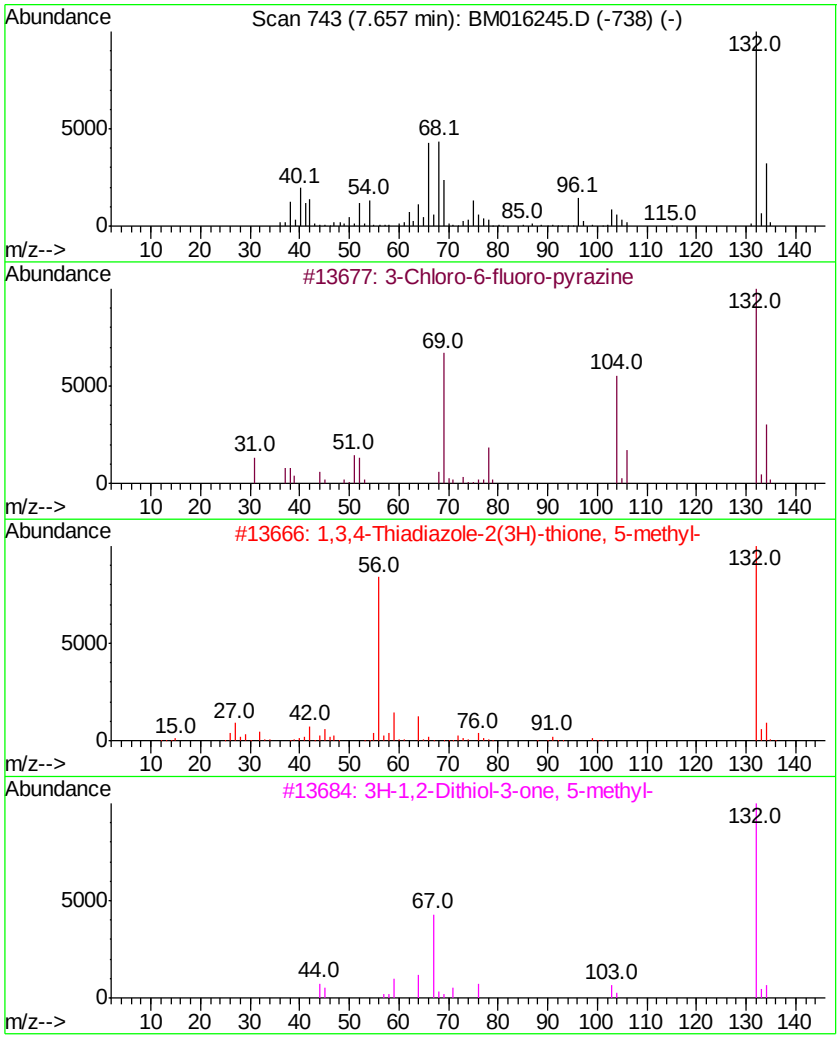
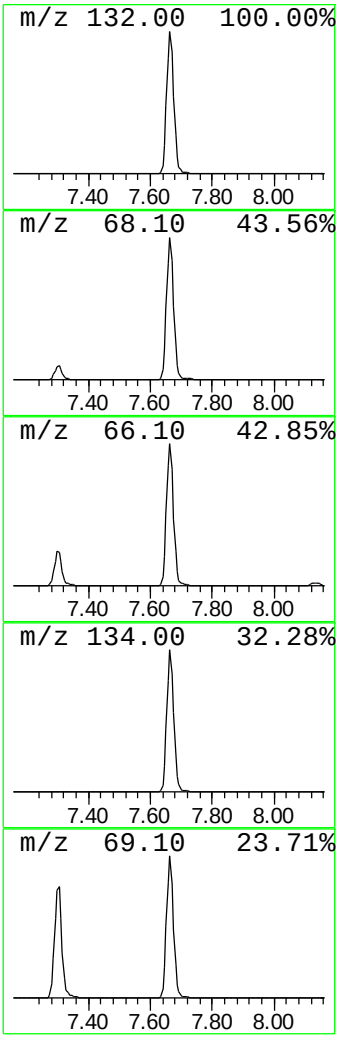
Peak Number 2 unknown7.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	90.63 ng	1355700	1,4-Dichlorobenzene-d4	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
2	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
3	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	12





Library Search Compound Report

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Data File : BM016245.D
Acq On : 08 Aug 2018 12:10
Operator : SJ/JU
Sample : J4327-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : FK-BPM-02-007-ABCD

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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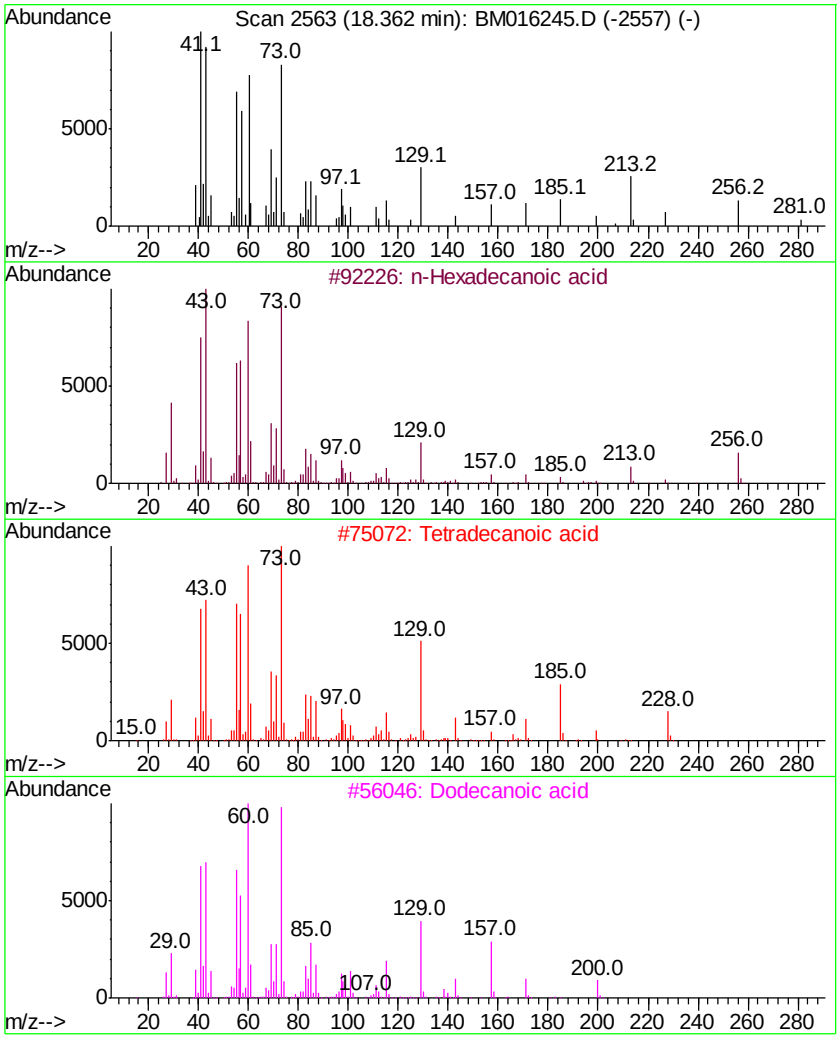
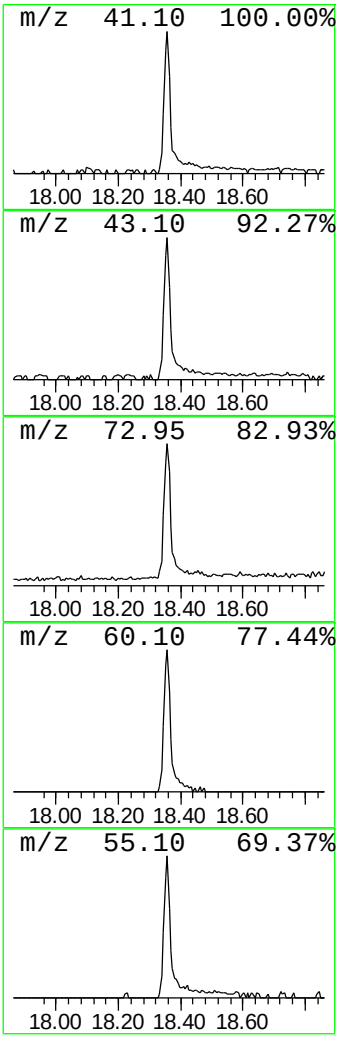
Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.36	9.25 ng	193620	Phenanthrene-d10	17.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
3	Dodecanoic acid	200	C12H24O2	000143-07-7	52
4	Undecanoic acid	186	C11H22O2	000112-37-8	50
5	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	47





Library Search Compound Report

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Data File : BM016245.D
Acq On : 08 Aug 2018 12:10
Operator : SJ/JU
Sample : J4327-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : FK-BPM-02-007-ABCD

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

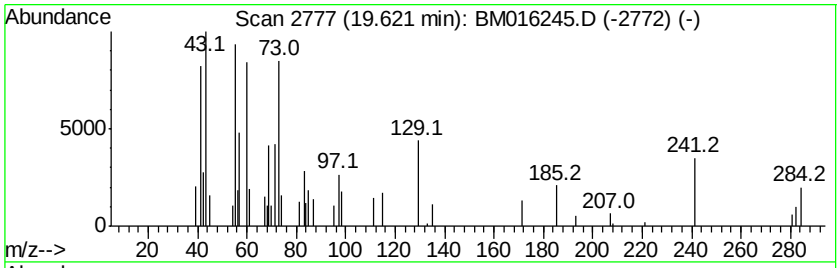
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

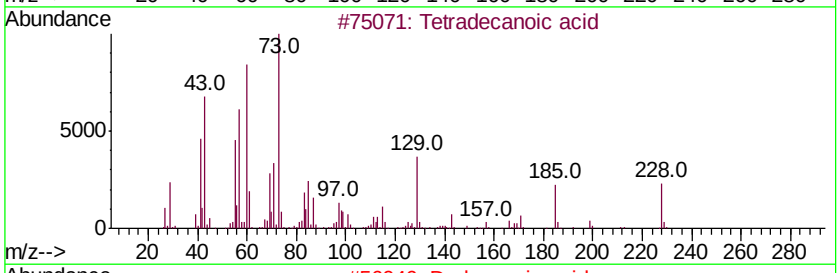
****

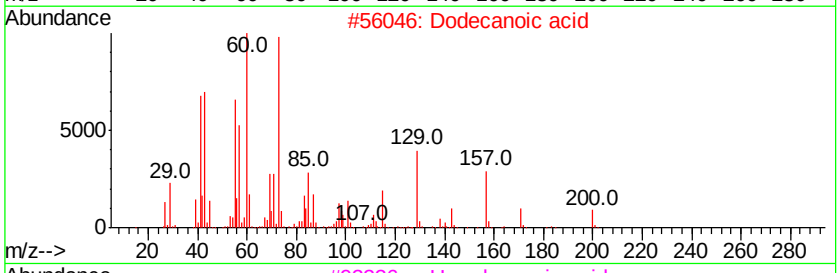
Peak Number 5 Tetradecanoic acid Concentration Rank 6

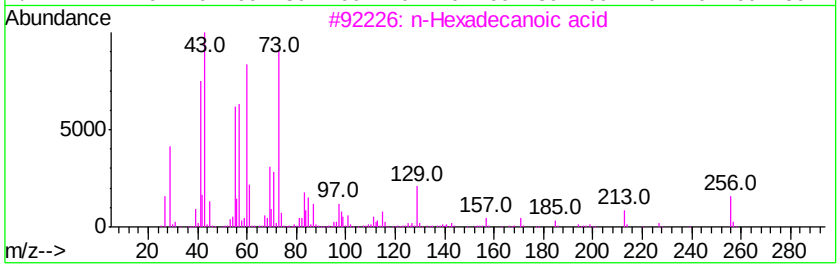
R.T.	EstConc	Area	Relative to ISTD	R.T.
19.62	3.43 ng	80952	Chrysene-d12	21.63

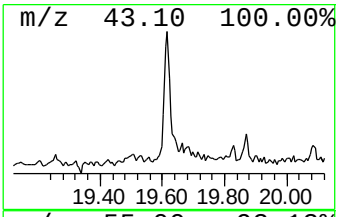
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
2	Dodecanoic acid	200	C12H24O2	000143-07-7	35
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	27
4	Tridecanoic acid	214	C13H26O2	000638-53-9	27
5	n-Decanoic acid	172	C10H20O2	000334-48-5	22

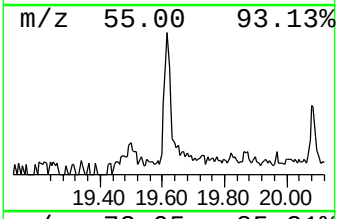


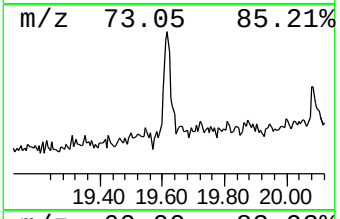


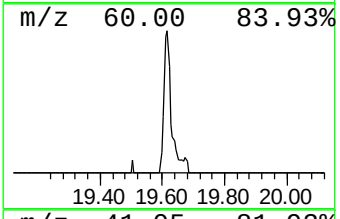


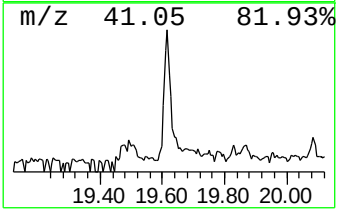












Library Search Compound Report

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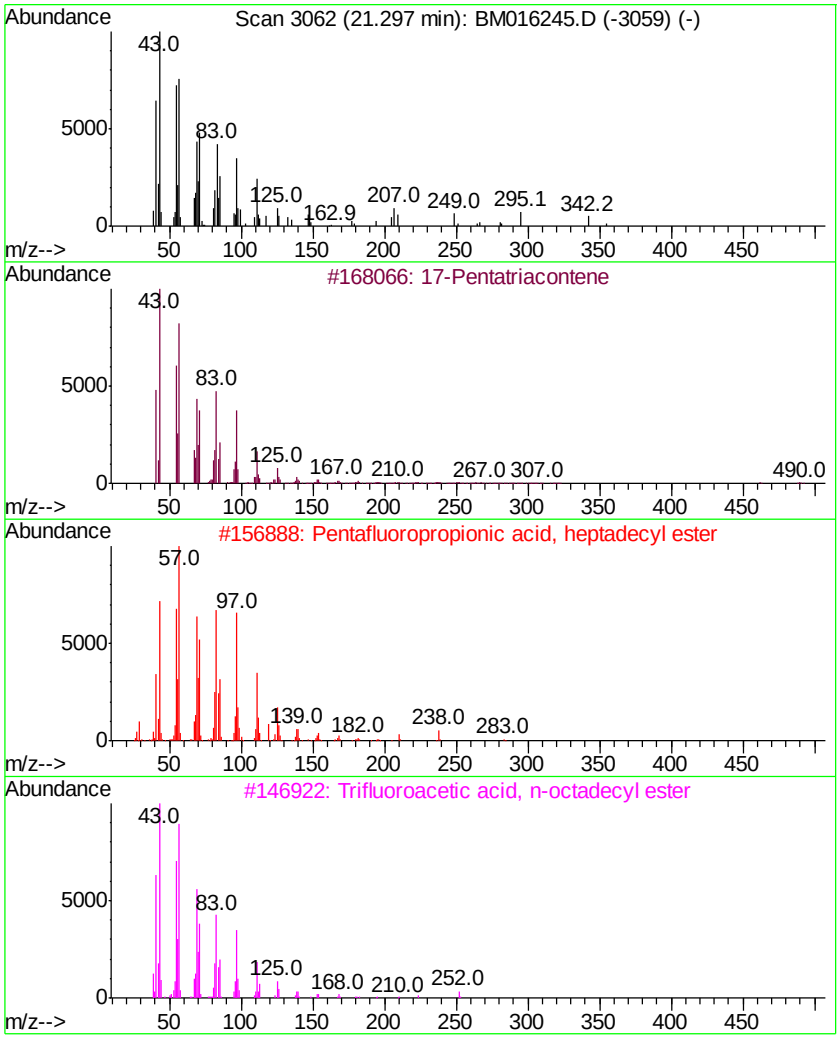
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

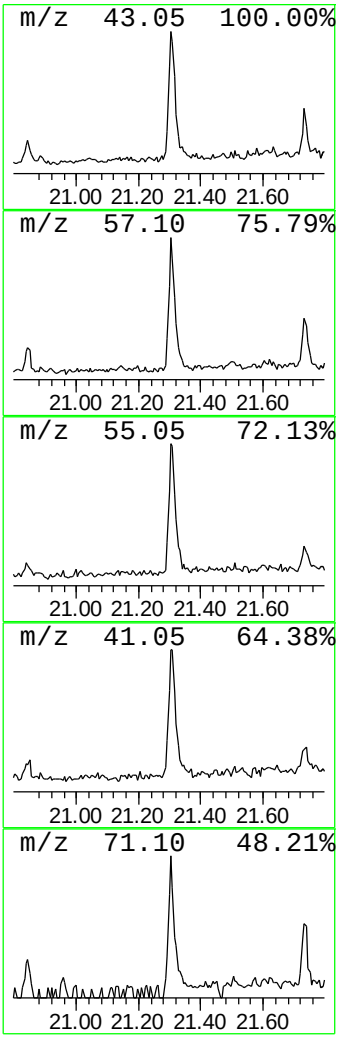
****

Peak Number 6 17-Pentatriacontene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.30	6.83 ng	161114	Chrysene-d12	21.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	87
2	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	87
3	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	87
4	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	87
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87





Tentatively Identified Compound (LSC) summary

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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...	5.19	11.6	ng	174045	1	8.13	299172	20.0
unknown7.66	7.66	90.6	ng	1355700	1	8.13	299172	20.0
n-Hexadecanoic acid	18.36	9.3	ng	193620	4	17.50	418482	20.0
Tetradecanoic acid	19.62	3.4	ng	80952	5	21.63	472008	20.0
17-Pentatriacontene	21.30	6.8	ng	161114	5	21.63	472008	20.0