LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM033017\
Data File : BM009455.D
Acq On : 30 Mar 2017 17:45
Operator : SJ/MA
Sample : I2445-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 032717-PRRT-F-D-M

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-BM032217.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	4.375	215	219	228	rBV	117510	158421	1.55%	0.377%
2	4.969	315	320	328	rVB	651245	889944	8.70%	2.115%
3	5.422	390	397	405	rBV	928146	1339084	13.09%	3.183%
4	6.040	497	502	508	rVB	116626	163820	1.60%	0.389%
5	7.005	660	666	676	rVB	532622	848077	8.29%	2.016%
6	7.381	722	730	737	rBV	1532331	2504466	24.48%	5.952%
7	7.852	801	810	817	rBV	484737	781692	7.64%	1.858%
8	8.169	857	864	872	rVB	2279323	3641362	35.60%	8.654%
9	9.016	1000	1008	1018	rBV	1978556	3204695	31.33%	7.616%
10	10.646	1279	1285	1293	rVB	588421	978205	9.56%	2.325%
11	13.110	1697	1704	1712	rBV	4445439	6320000	61.78%	15.020%
12	13.945	1841	1846	1852	rBV	107986	154122	1.51%	0.366%
13	14.492	1933	1939	1947	rBV3	797367	1229829	12.02%	2.923%
14	15.986	2187	2193	2208	rVB	2124833	3097185	30.28%	7.361%
15	16.186	2222	2227	2236	rBV2	62765	119738	1.17%	0.285%
16	17.239	2400	2406	2416	rBV	1064027	1575441	15.40%	3.744%
17	18.116	2549	2555	2562	rBV2	113149	168574	1.65%	0.401%
18	19.392	2768	2772	2783	rBV2	91966	140977	1.38%	0.335%
19	19.863	2845	2852	2863	rBV	7982297	10229695	100.00%	24.312%
20	21.104	3059	3063	3069	rBV2	181176	249913	2.44%	0.594%
21	21.415	3111	3116	3121	rBV	1785302	2193748	21.44%	5.214%
22	23.739	3505	3511	3522	rVB2	1012587	2087112	20.40%	4.960%

Sum of corrected areas: 42076100

LSC Report - Integrated Chromatogram

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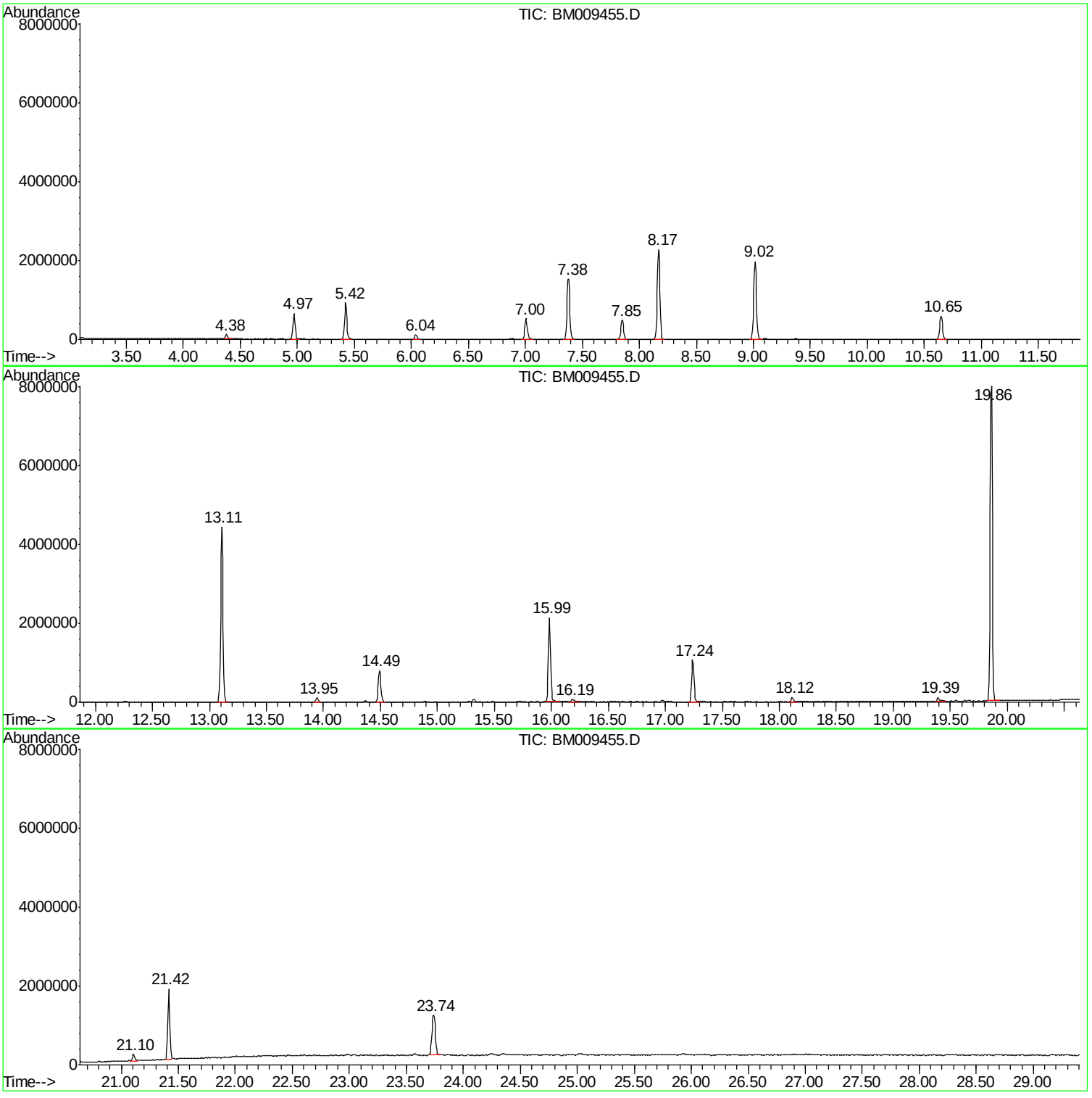
Instrument : BNA_M
ClientSampleId : 032717-PRRT-F-D-M

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM032217.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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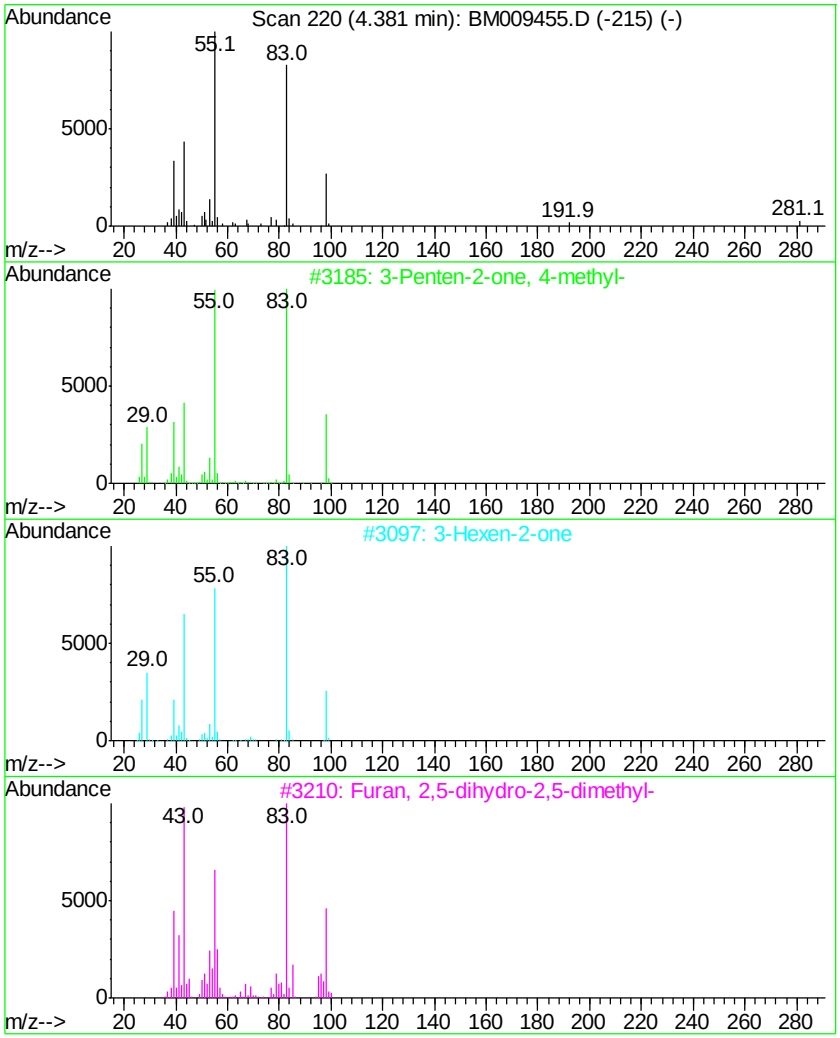
TIC Integration Parameters: LSCINT.P

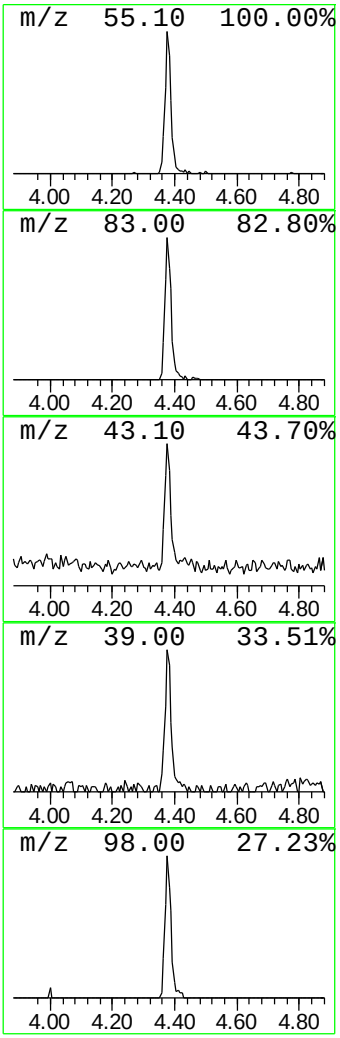
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.38	4.05 ng	158421	1,4-Dichlorobenzene-d4	7.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
2	3-Hexen-2-one	98	C6H10O	000763-93-9	80
3	Furan, 2,5-dihydro-2,5-dimethyl-	98	C6H10O	059242-27-2	80
4	2-Pentene, 4,4-dimethyl-	98	C7H14	026232-98-4	78
5	3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	64





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Instrument : BNA_M
ClientSampleId : 032717-PRRT-F-D-M

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM032217.M
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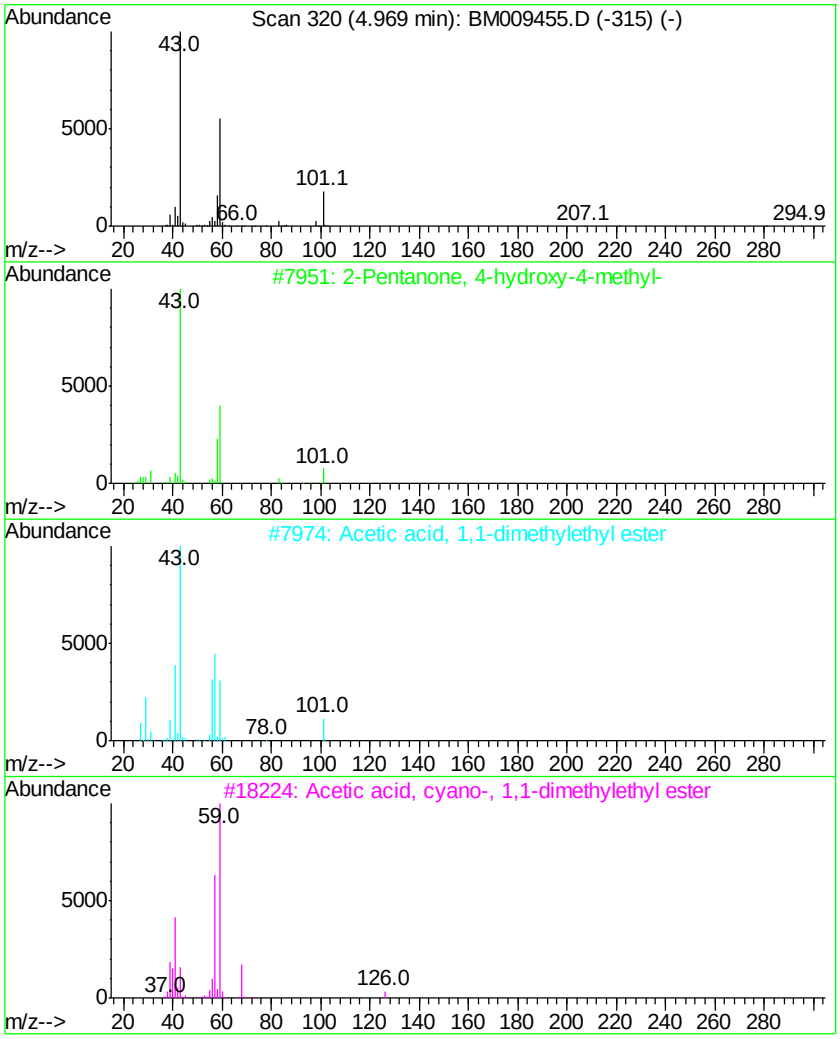
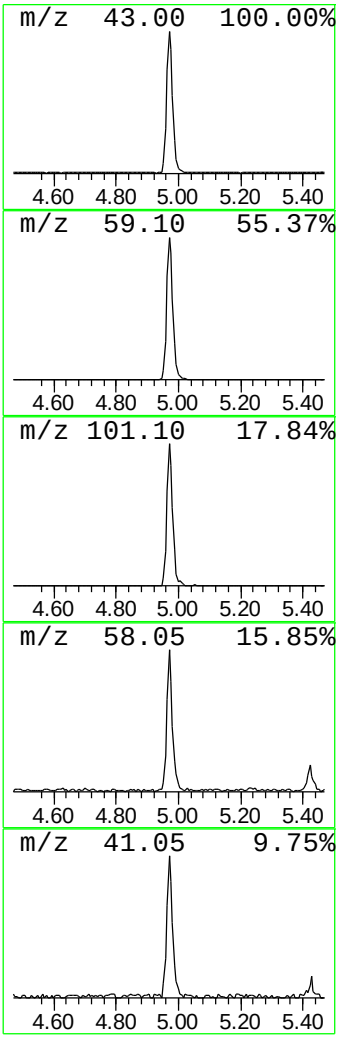
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	22.77 ng	889944	1,4-Dichlorobenzene-d4	7.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Acetic acid, 2-propenyl ester	100	C5H8O2	000591-87-7	9





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Sample : I2445-01
Misc :
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Instrument : BNA_M
ClientSampleId : 032717-PRRT-F-D-M

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM032217.M
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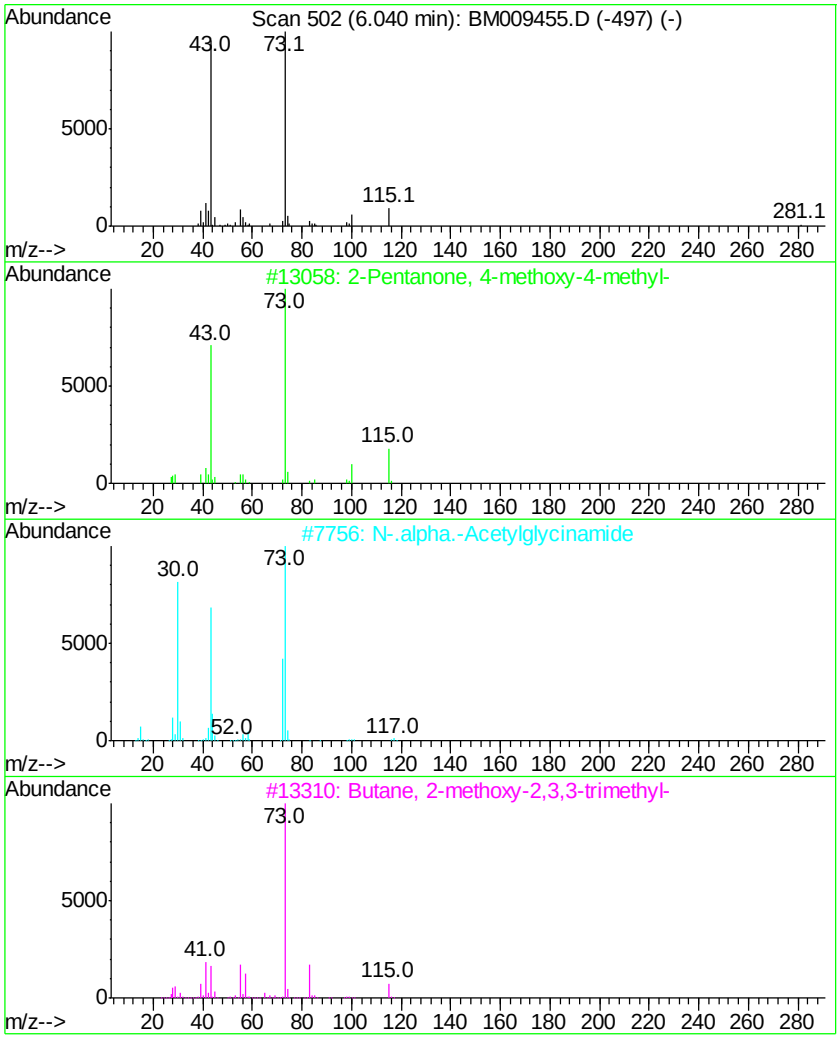
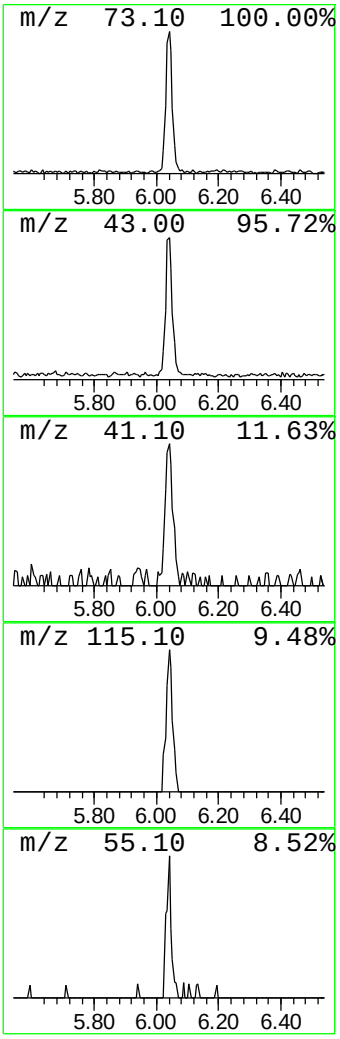
Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.04	4.19 ng	163820	1,4-Dichlorobenzene-d4	7.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	78
2	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	28
3	Butane, 2-methoxy-2,3,3-trimethyl-	130	C8H18O	027705-21-1	25
4	N-Ethylformamide	73	C3H7NO	000627-45-2	12
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	10





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Sample : I2445-01
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Instrument : BNA_M
ClientSampleId : 032717-PRRT-F-D-M

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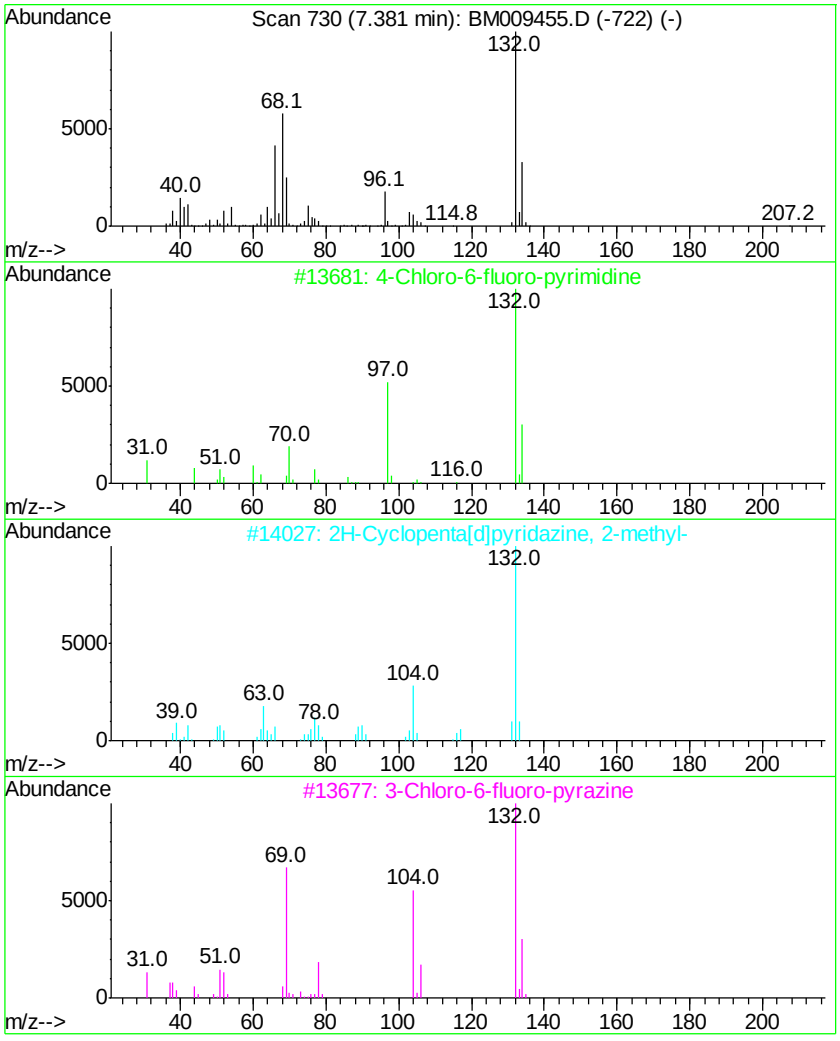
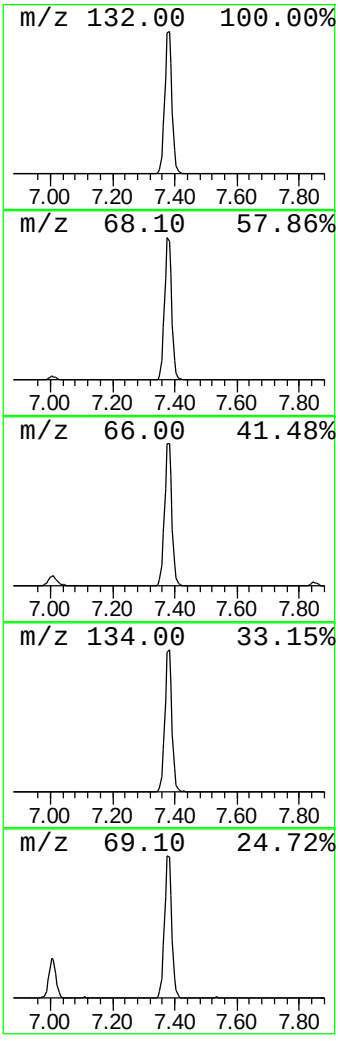
Peak Number 4 unknown7.38 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.38	64.08 ng	2504470	1,4-Dichlorobenzene-d4	7.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
2	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	14
3	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	10
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	10





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Instrument : BNA_M
ClientSampleId : 032717-PRRT-F-D-M

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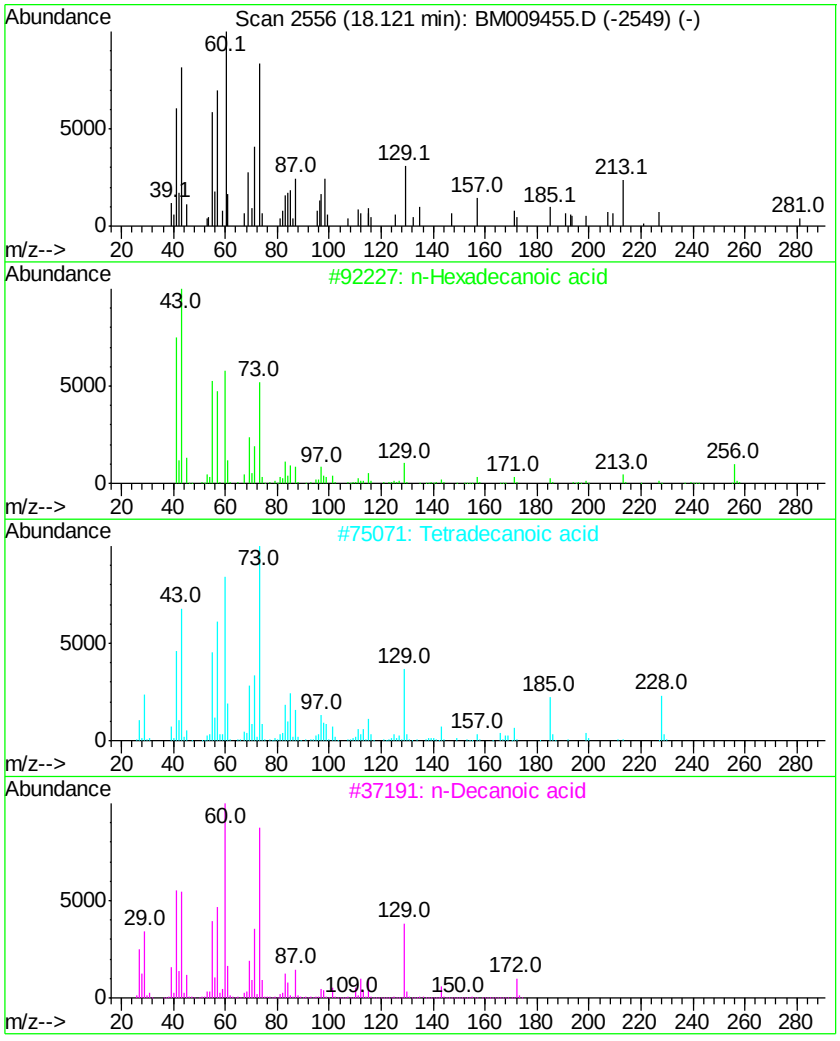
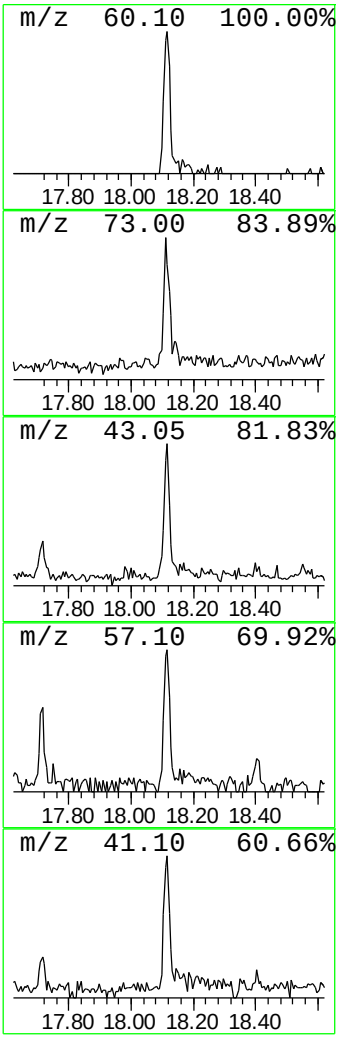
Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.12	2.14 ng	168574	Phenanthrene-d10	17.24

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	50
3	n-Decanoic acid	172	C10H20O2	000334-48-5	43
4	Dodecanoic acid	200	C12H24O2	000143-07-7	30
5	Tridecanoic acid	214	C13H26O2	000638-53-9	30





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Instrument : BNA_M
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Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM032217.M
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TIC Integration Parameters: LSCINT.P

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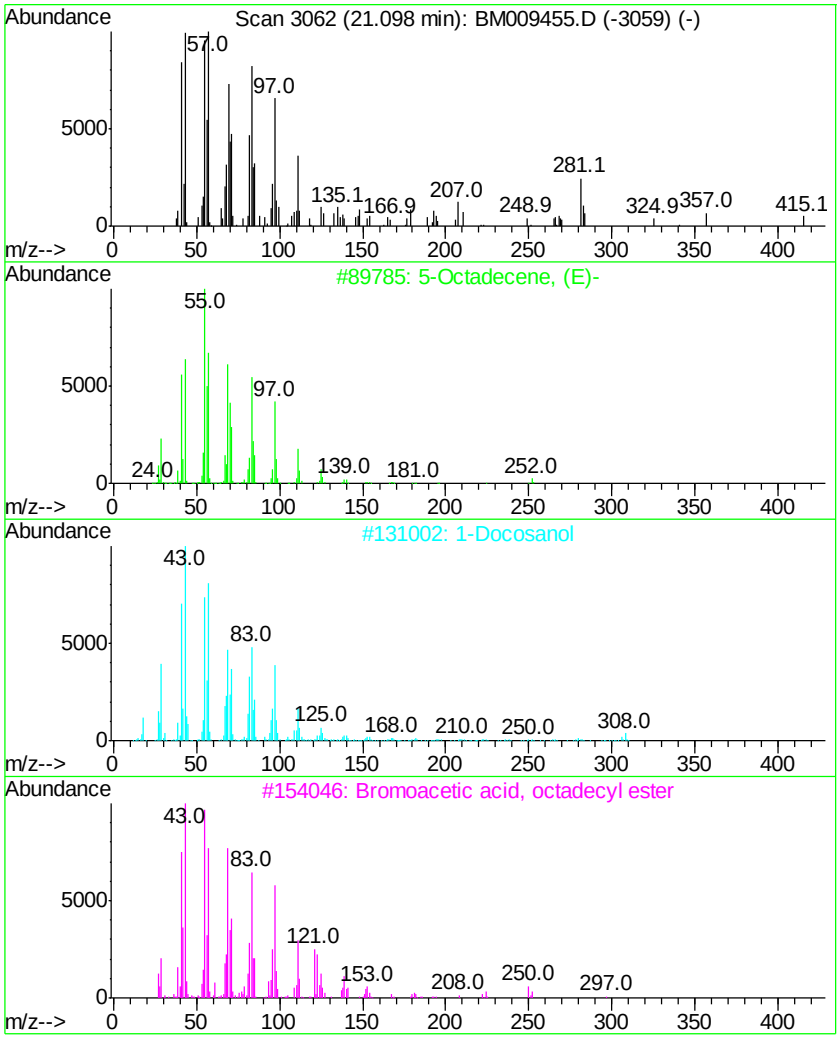
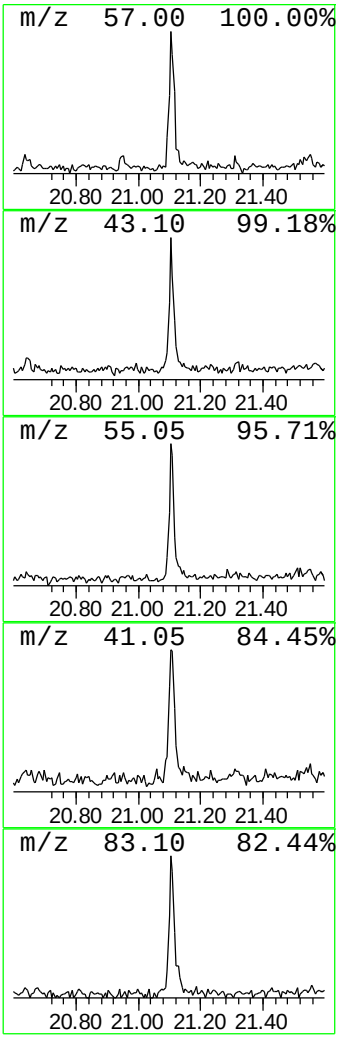
Peak Number 7 5-Octadecene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.10	2.28 ng	249913	Chrysene-d12	21.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	93
2	1-Docosanol	326	C22H46O	000661-19-8	91
3	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
4	1-Octadecene	252	C18H36	000112-88-9	91
5	Z-5-Nonadecene	266	C19H38	1000131-11-8	91





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
3-Penten-2-one, 4...	4.38	4.0	ng	158421	1	7.85	781692	20.0
2-Pentanone, 4-hy...	4.97	22.8	ng	889944	1	7.85	781692	20.0
2-Pentanone, 4-me...	6.04	4.2	ng	163820	1	7.85	781692	20.0
unknown7.38	7.38	64.1	ng	2504470	1	7.85	781692	20.0
n-Hexadecanoic acid	18.12	2.1	ng	168574	4	17.24	1575440	20.0
5-Octadecene, (E)-	21.10	2.3	ng	249913	5	21.42	2193750	20.0