LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121618\
Data File : BM018228.D
Acq On : 16 Dec 2018 16:03
Operator : JU/SJ
Sample : J6377-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P001-SD004-0006-01

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	4.687	302	306	316	rVB	62005	83245	2.92%	0.325%
2	5.128	375	381	402	rBV	1719696	2451544	86.00%	9.558%
3	6.693	641	647	665	rBV	1540081	2645910	92.81%	10.316%
4	7.034	699	705	719	rBV	1697708	2696940	94.60%	10.515%
5	7.498	778	784	792	rBV	392953	630062	22.10%	2.456%
6	7.810	829	837	848	rBV	1227460	1928400	67.65%	7.518%
7	8.657	973	981	995	rBV	835441	1514404	53.12%	5.904%
8	10.263	1246	1254	1273	rBV	408478	810661	28.44%	3.161%
9	12.763	1672	1679	1694	rBV	1741151	2800626	98.24%	10.919%
10	13.639	1822	1828	1837	rBV	73689	131816	4.62%	0.514%
11	14.157	1909	1916	1929	rBV2	587240	966745	33.91%	3.769%
12	15.663	2166	2172	2183	rBV	1265073	2011267	70.55%	7.841%
13	16.915	2378	2385	2396	rBV2	620501	1018423	35.72%	3.971%
14	17.827	2536	2540	2553	rBV2	65885	113845	3.99%	0.444%
15	19.127	2755	2761	2766	rBV6	32789	53936	1.89%	0.210%
16	19.568	2831	2836	2848	rBV	2255677	2850749	100.00%	11.114%
17	20.862	3052	3056	3062	rBV2	88321	135118	4.74%	0.527%
18	21.139	3098	3103	3112	rBV	857131	1159381	40.67%	4.520%
19	21.721	3199	3202	3204	rBV4	79749	88196	3.09%	0.344%
20	21.756	3204	3208	3213	rVB3	159013	238954	8.38%	0.932%
21	22.650	3356	3360	3365	rVB	147754	199449	7.00%	0.778%
22	23.297	3464	3470	3479	rVB	613011	1119423	39.27%	4.364%

Sum of corrected areas: 25649094

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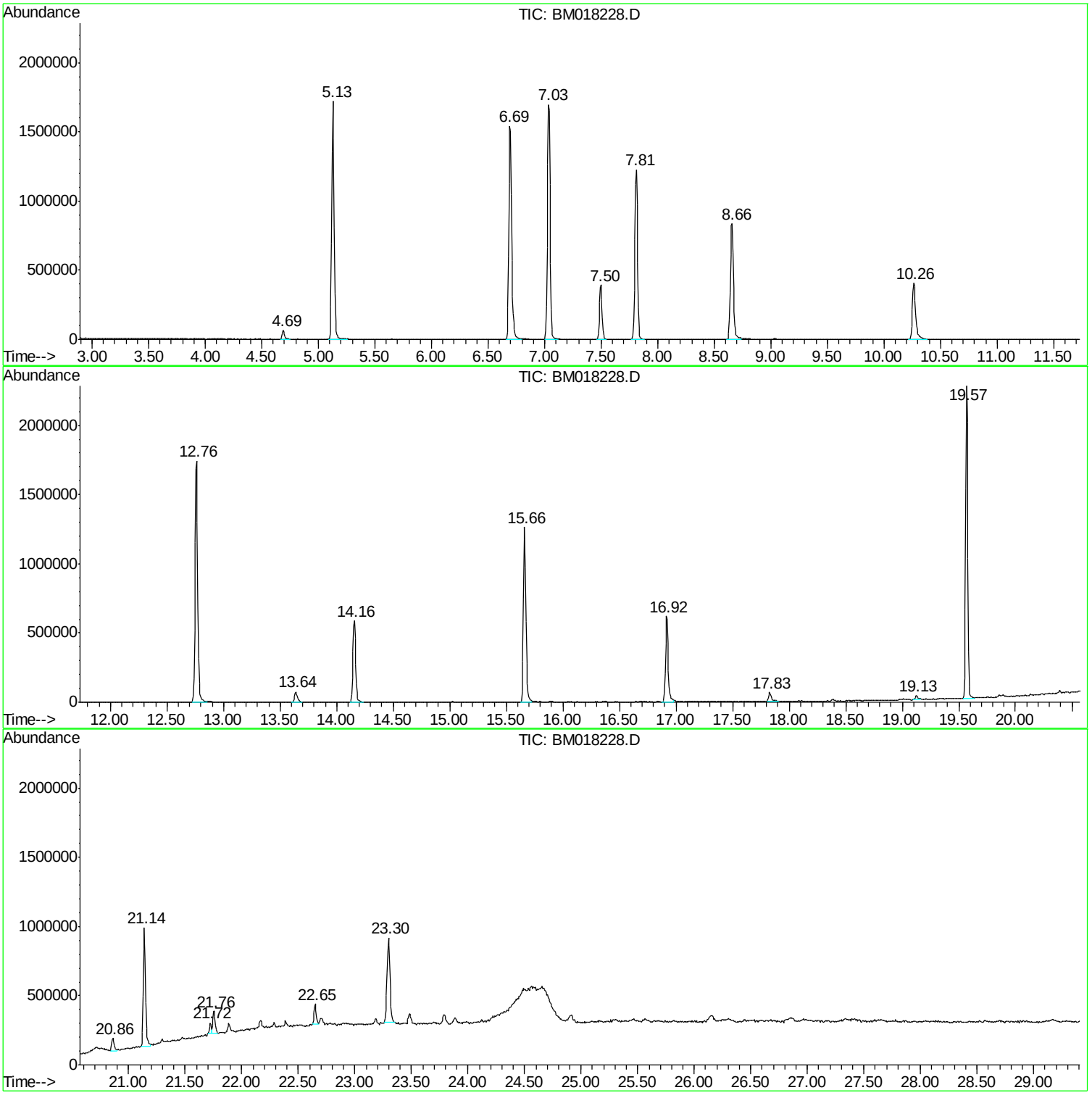
Instrument :
BNA_M
ClientSampleId :
P001-SD004-0006-01

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\BM121618\
Data File : BM018228.D
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Operator : JU/SJ
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Misc :
ALS Vial : 10 Sample Multiplier: 1

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

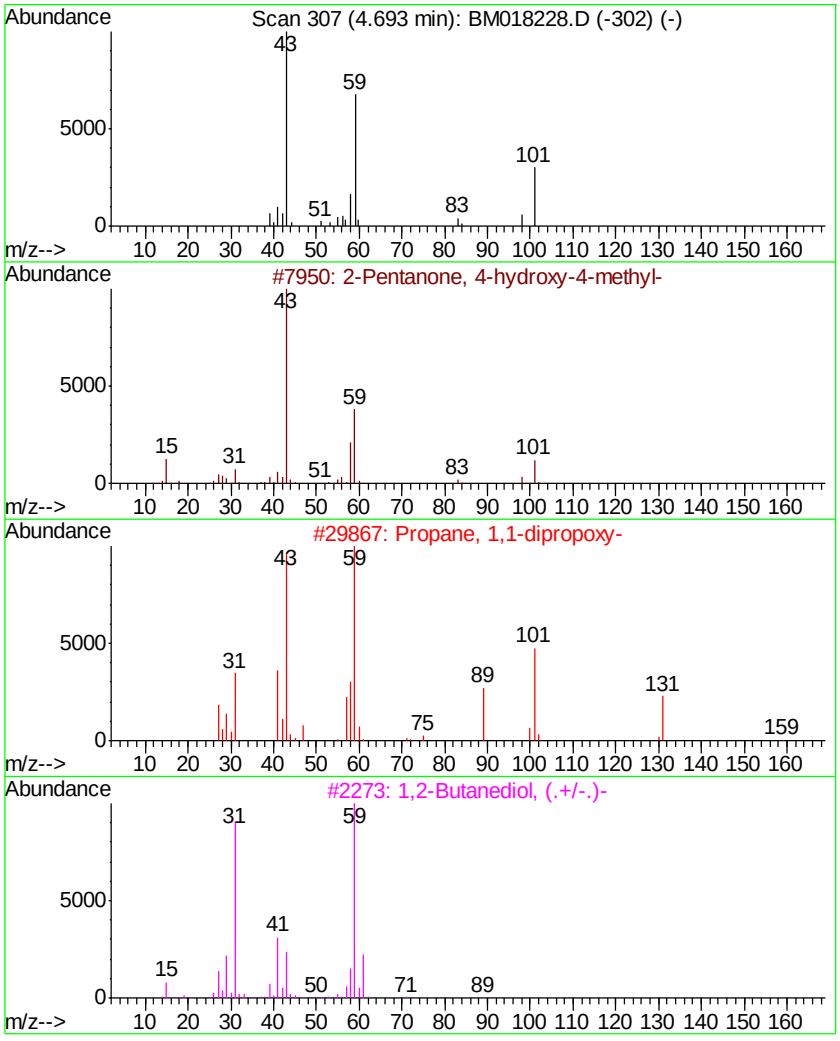
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

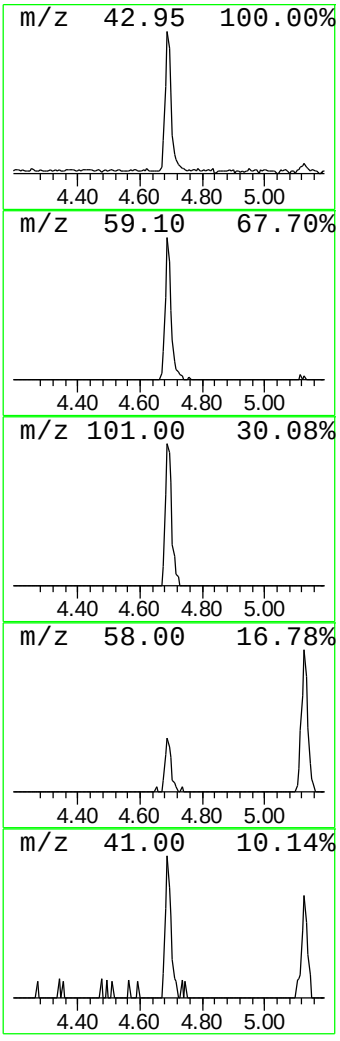
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.69	2.64 ng	83245	1,4-Dichlorobenzene-d4	7.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 1,1-dipropoxy-	160	C9H20O2	004744-11-0	45
3	1,2-Butanediol, (.+/-.)-	90	C4H10O2	026171-83-5	32
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	28
5	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25





Library Search Compound Report

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Instrument : BNA_M
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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
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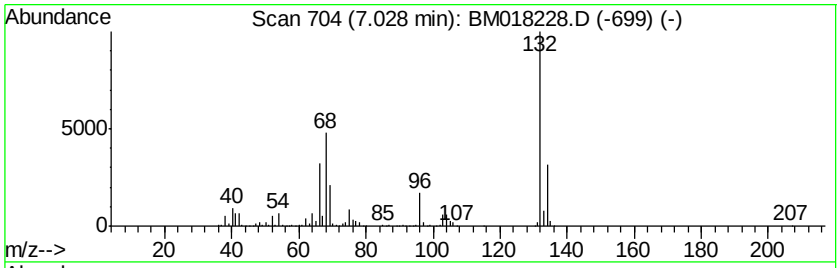
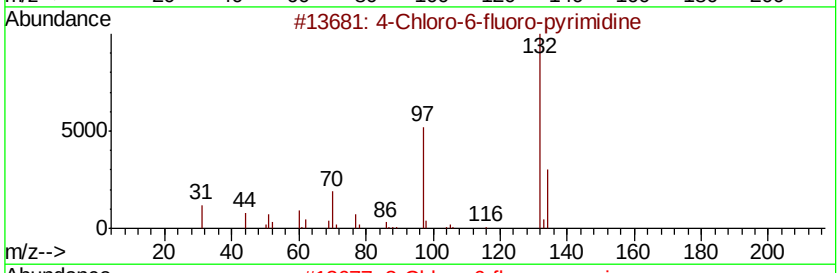
****

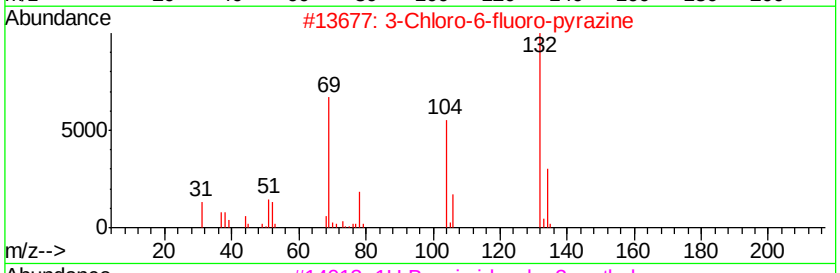
Peak Number 2 unknown7.03 Concentration Rank 1

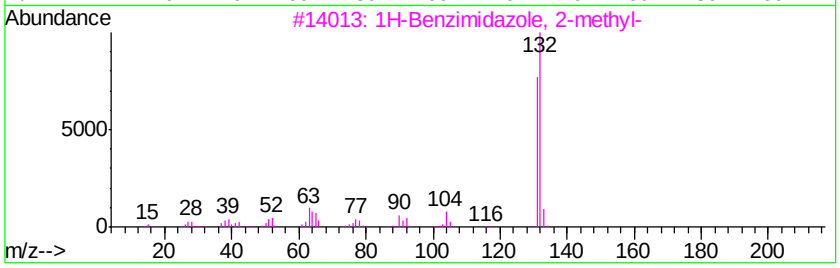
R.T.	EstConc	Area	Relative to ISTD	R.T.
7.03	85.61 ng	2696940	1,4-Dichlorobenzene-d4	7.50

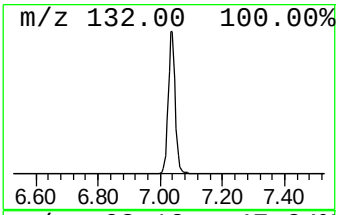
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	5-Aminoindole	132	C8H8N2	005192-03-0	10

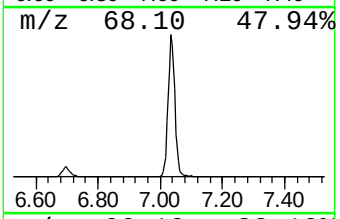


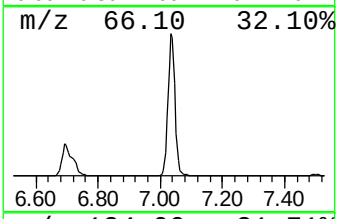


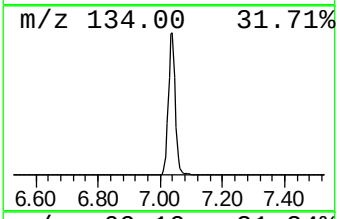


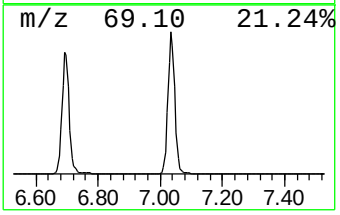












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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P001-SD004-0006-01

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

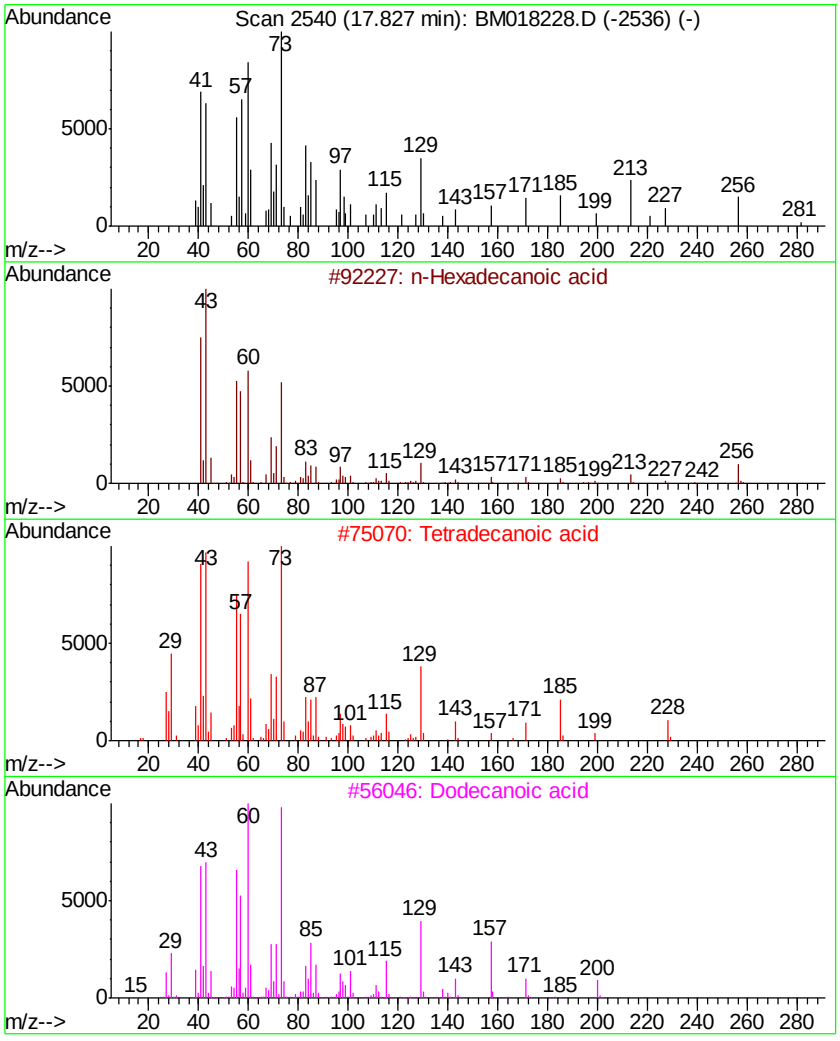
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

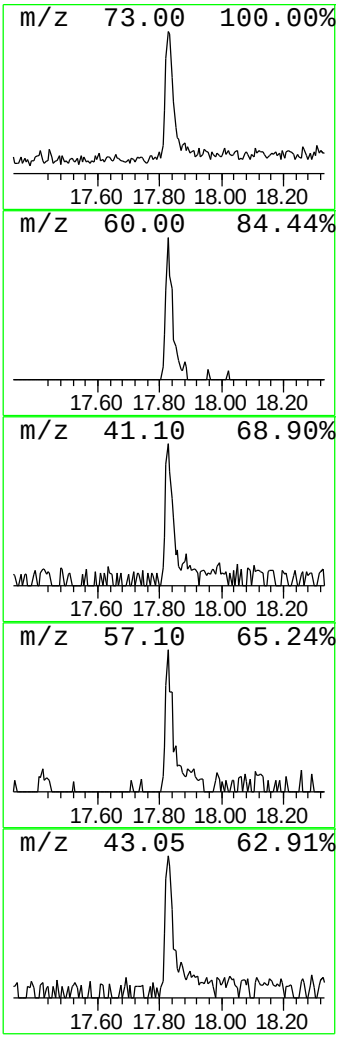
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.83	2.24 ng	113845	Phenanthrene-d10	16.92

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	52
3	Dodecanoic acid	200	C12H24O2	000143-07-7	49
4	Tridecanoic acid	214	C13H26O2	000638-53-9	47
5	n-Decanoic acid	172	C10H20O2	000334-48-5	38





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Instrument : BNA_M
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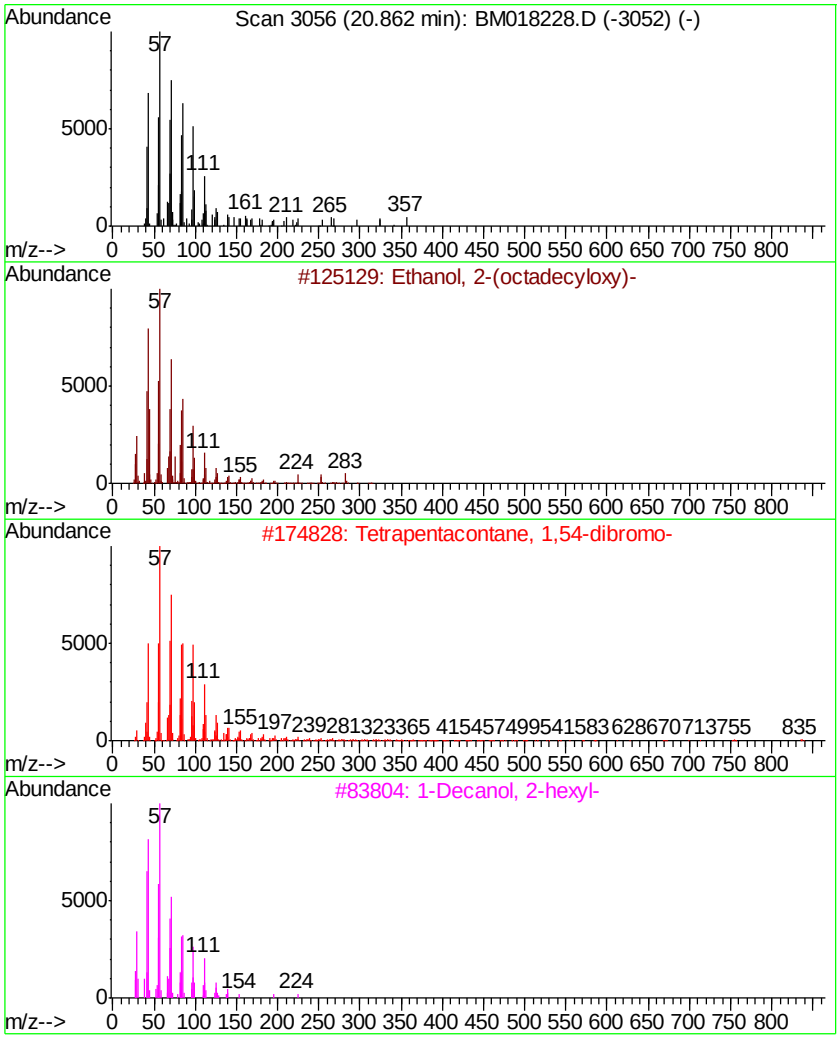
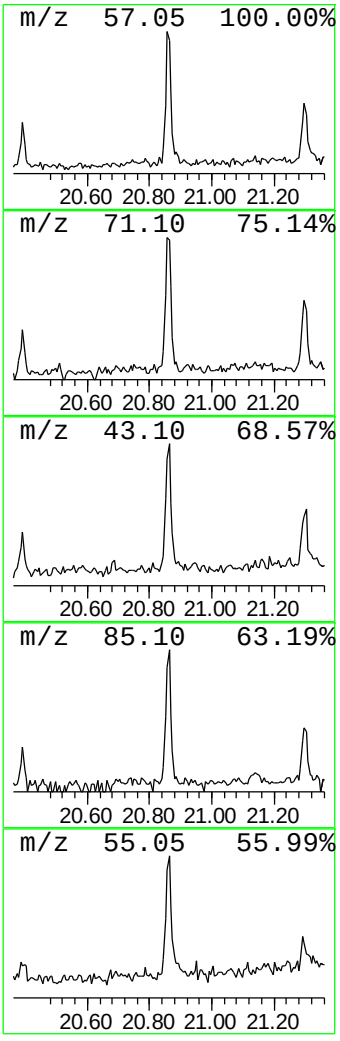
****

Peak Number 5 Ethanol, 2-(octadecyloxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.86	2.33 ng	135118	Chrysene-d12	21.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(octadecyloxy)-	314	C20H42O2	002136-72-3	86
2	Tetrapentacontane, 1,54-dibromo-	915	C54H108Br2	1000156-09-4	74
3	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	68
4	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	52
5	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	50





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Instrument : BNA_M
ClientSampleId : P001-SD004-0006-01

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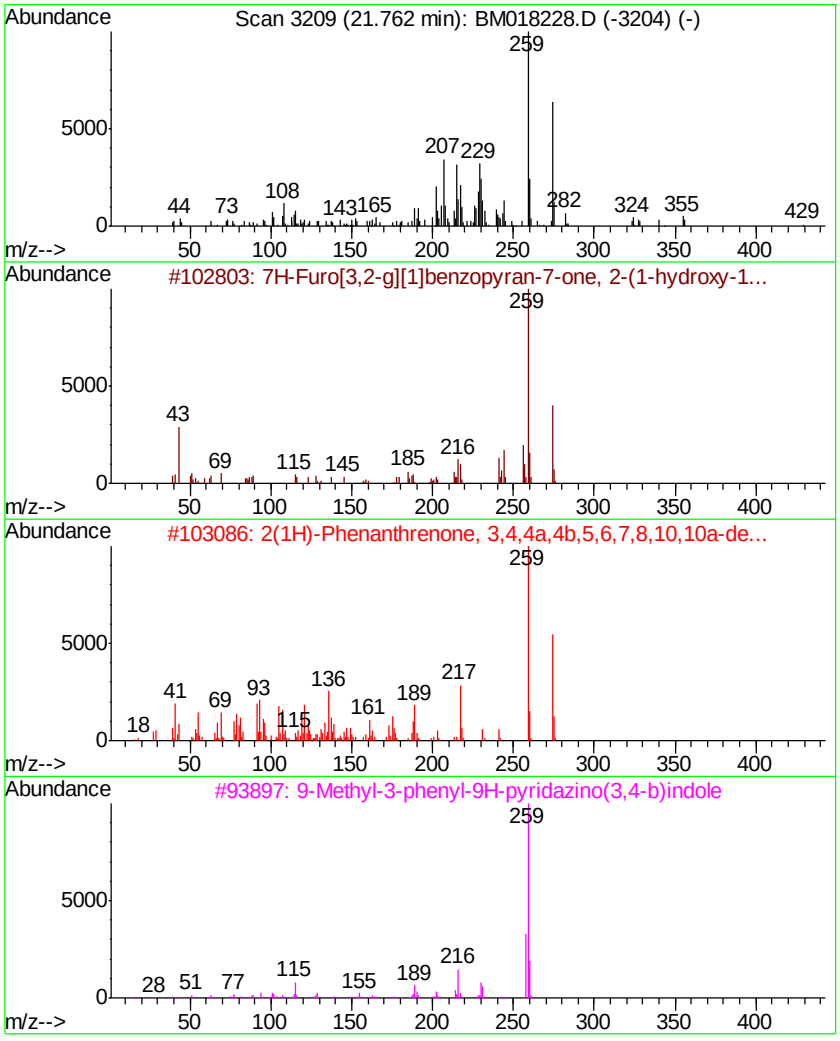
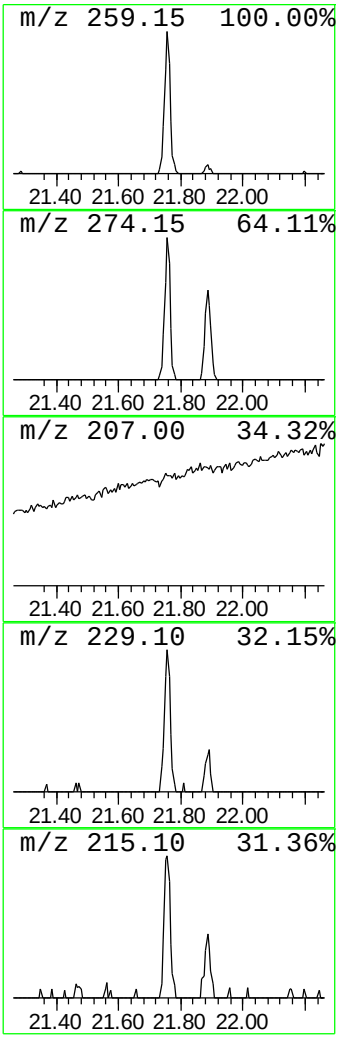
****

Peak Number 6 7H-Furo[3,2-g][1]benzopyran... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.76	4.12 ng	238954	Chrysene-d12	21.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7H-Furo[3,2-g][1]benzopyran-7-on...	274	C15H14O5	054087-32-0	64
2	2(1H)-Phenanthrenone, 3,4,4a,4b,...	274	C19H30O	007715-44-8	49
3	9-Methyl-3-phenyl-9H-pyridazino(...	259	C17H13N3	003980-90-3	38
4	Benz[a]anthracen-7(12H)-one, 12-...	274	C19H14O2	017513-39-2	38
5	[2](1,4)Naphthaleno[2](2,6)pyrid...	259	C19H17N	099677-63-1	38





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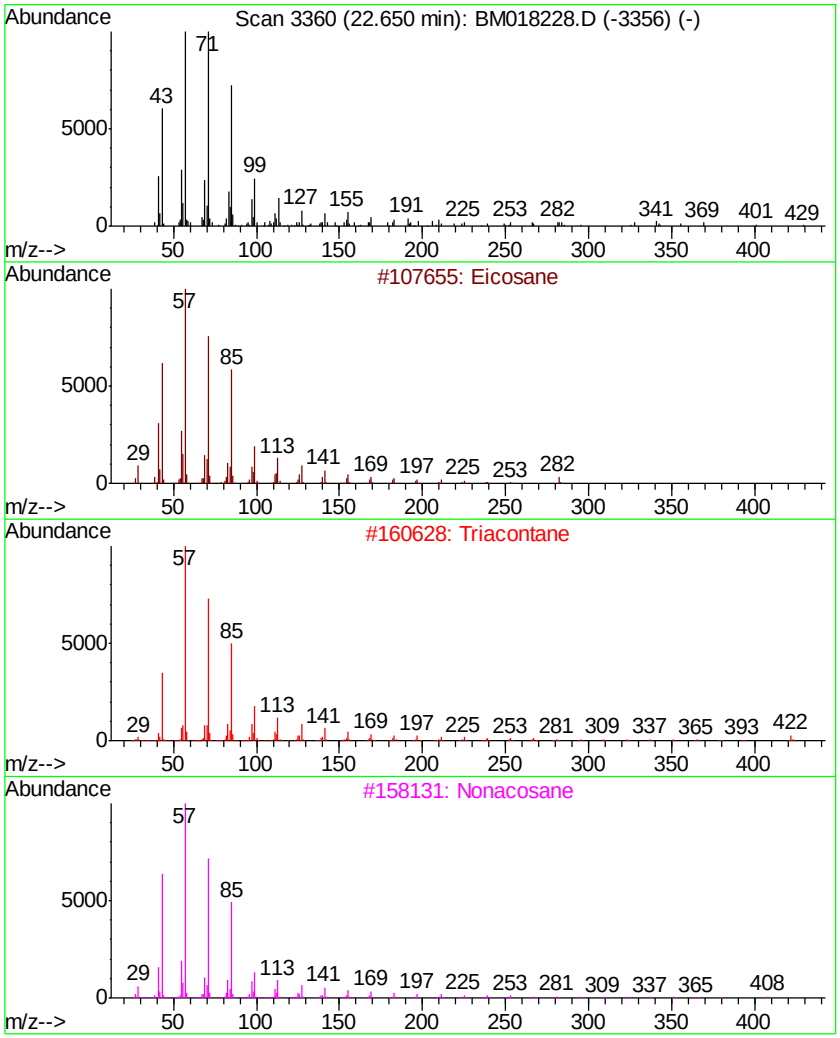
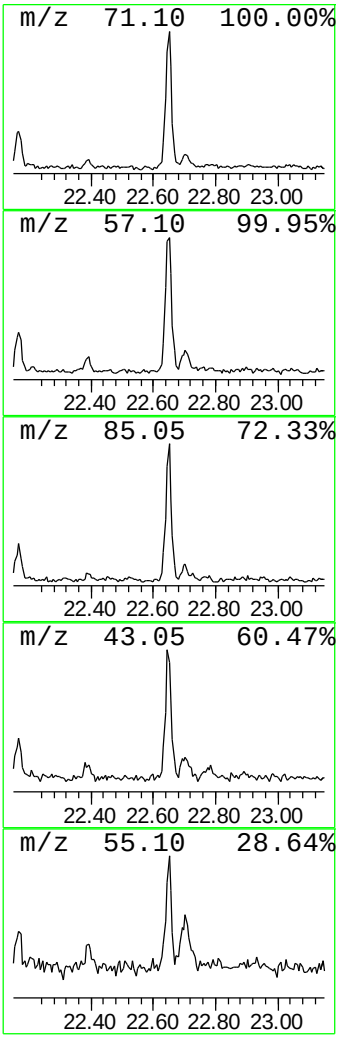
****

Peak Number 7 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.65	3.56 ng	199449	Perylene-d12	23.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	90
2	Triacontane	422	C30H62	000638-68-6	87
3	Nonacosane	408	C29H60	000630-03-5	83
4	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	80
5	Docosane, 9-butyl-	366	C26H54	055282-14-9	80





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...	4.69	2.6	ng	83245	1	7.50	630062	20.0
unknown7.03	7.03	85.6	ng	2696940	1	7.50	630062	20.0
n-Hexadecanoic acid	17.83	2.2	ng	113845	4	16.92	1018420	20.0
Ethanol, 2-(octad...	20.86	2.3	ng	135118	5	21.14	1159380	20.0
7H-Furo[3,2-g][1]...	21.76	4.1	ng	238954	5	21.14	1159380	20.0
Eicosane	22.65	3.6	ng	199449	6	23.30	1119420	20.0