LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011619\
Data File : BM018588.D
Acq On : 16 Jan 2019 18:02
Operator : JU/SJ
Sample : K1149-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SW002-190114-01

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-BM010919.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	3.705	101	105	121	rBV	53298	150721	5.21%	1.182%
2	5.340	376	383	394	rVB	245710	442444	15.30%	3.470%
3	6.922	646	652	662	rVB	218316	380370	13.15%	2.983%
4	7.281	704	713	724	rBV	517097	875505	30.27%	6.866%
5	7.746	787	792	802	rVB	119421	203890	7.05%	1.599%
6	8.063	839	846	853	rBV	420559	700341	24.21%	5.492%
7	8.910	984	990	999	rBV	319701	565512	19.55%	4.435%
8	10.539	1260	1267	1273	rBV	167927	275994	9.54%	2.164%
9	11.398	1405	1413	1420	rVB2	33689	73709	2.55%	0.578%
10	13.010	1680	1687	1697	rBV	983456	1421980	49.16%	11.151%
11	13.269	1727	1731	1737	rVB4	26906	44000	1.52%	0.345%
12	14.127	1868	1877	1881	rBV	56808	100098	3.46%	0.785%
13	14.257	1894	1899	1914	rVB	72694	178749	6.18%	1.402%
14	14.392	1917	1922	1930	rVB2	232451	373273	12.90%	2.927%
15	15.886	2169	2176	2188	rBV	846182	1223327	42.29%	9.593%
16	17.145	2385	2390	2395	rBV	350611	488130	16.88%	3.828%
17	18.027	2536	2540	2549	rBV2	141179	235347	8.14%	1.846%
18	18.562	2629	2631	2636	rBV5	17966	30001	1.04%	0.235%
19	19.209	2736	2741	2745	rBV6	24137	46607	1.61%	0.365%
20	19.309	2753	2758	2766	rBV2	109022	218793	7.56%	1.716%
21	19.774	2832	2837	2843	rBV	2531924	2892612	100.00%	22.684%
22	21.333	3098	3102	3108	rBV	609684	781803	27.03%	6.131%
23	22.509	3299	3302	3308	rVB	286171	380689	13.16%	2.985%
24	23.609	3486	3489	3498	rVB	357995	668035	23.09%	5.239%

Sum of corrected areas: 12751930

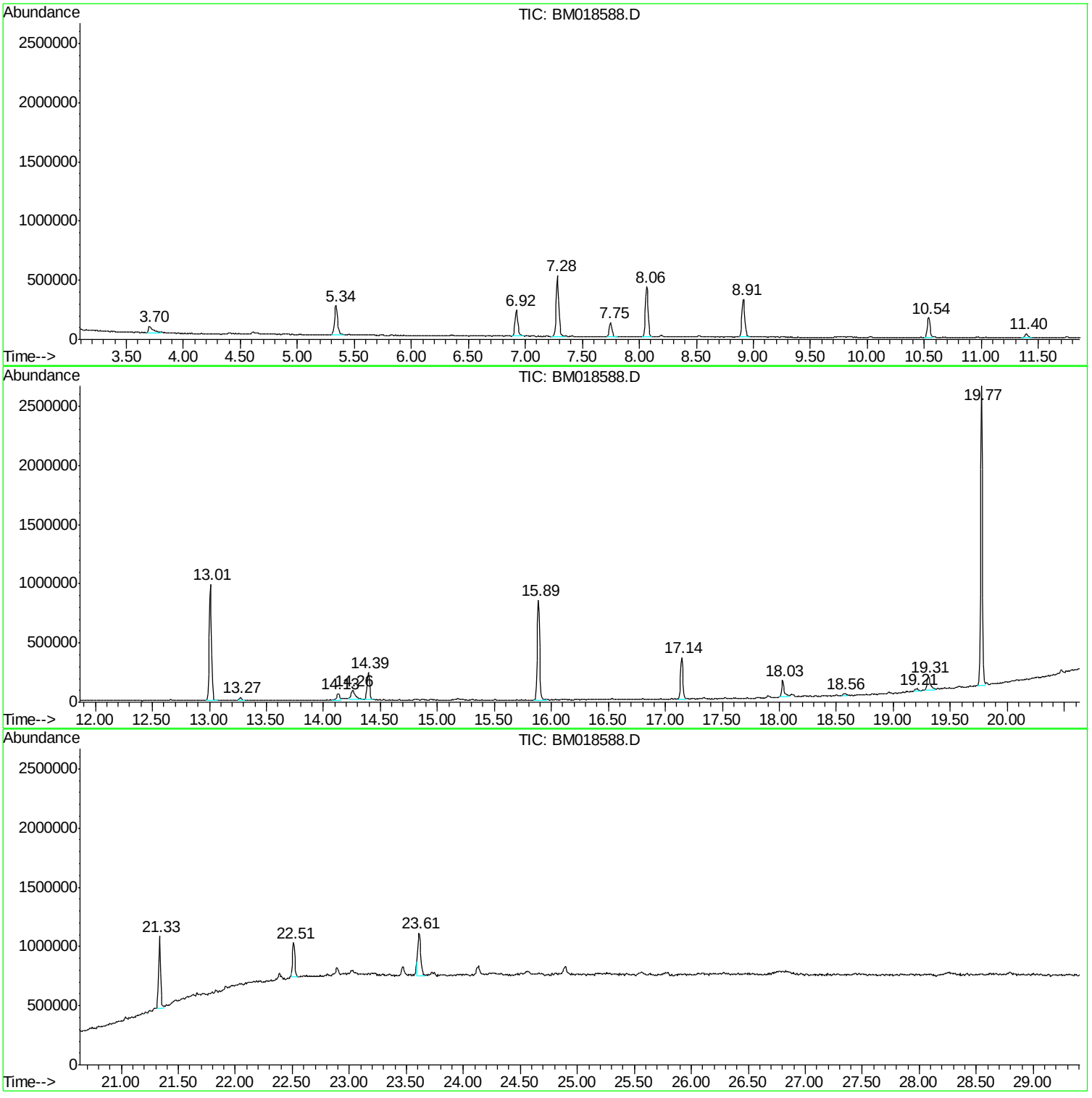
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011619\
Data File : BM018588.D
Acq On : 16 Jan 2019 18:02
Operator : JU/SJ
Sample : K1149-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SW002-190114-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.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\BM011619\
Data File : BM018588.D
Acq On : 16 Jan 2019 18:02
Operator : JU/SJ
Sample : K1149-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SW002-190114-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

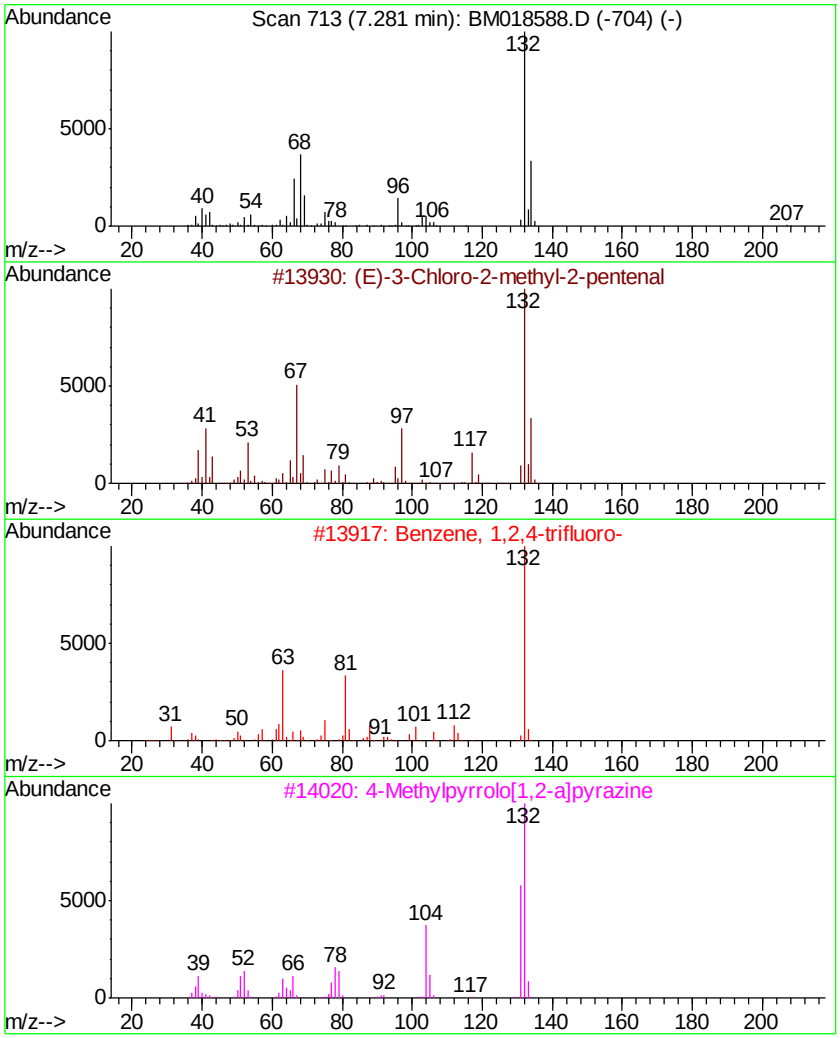
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

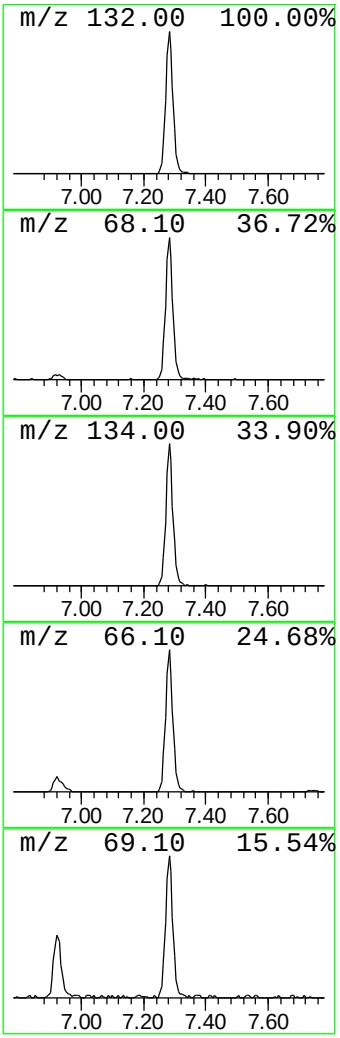
****

Peak Number 1 unknown7.28 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.28	85.88 ng	875505	1,4-Dichlorobenzene-d4	7.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
2	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
3	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
4	5-Aminoindole	132	C8H8N2	005192-03-0	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Library Search Compound Report

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Acq On : 16 Jan 2019 18:02
Operator : JU/SJ
Sample : K1149-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SW002-190114-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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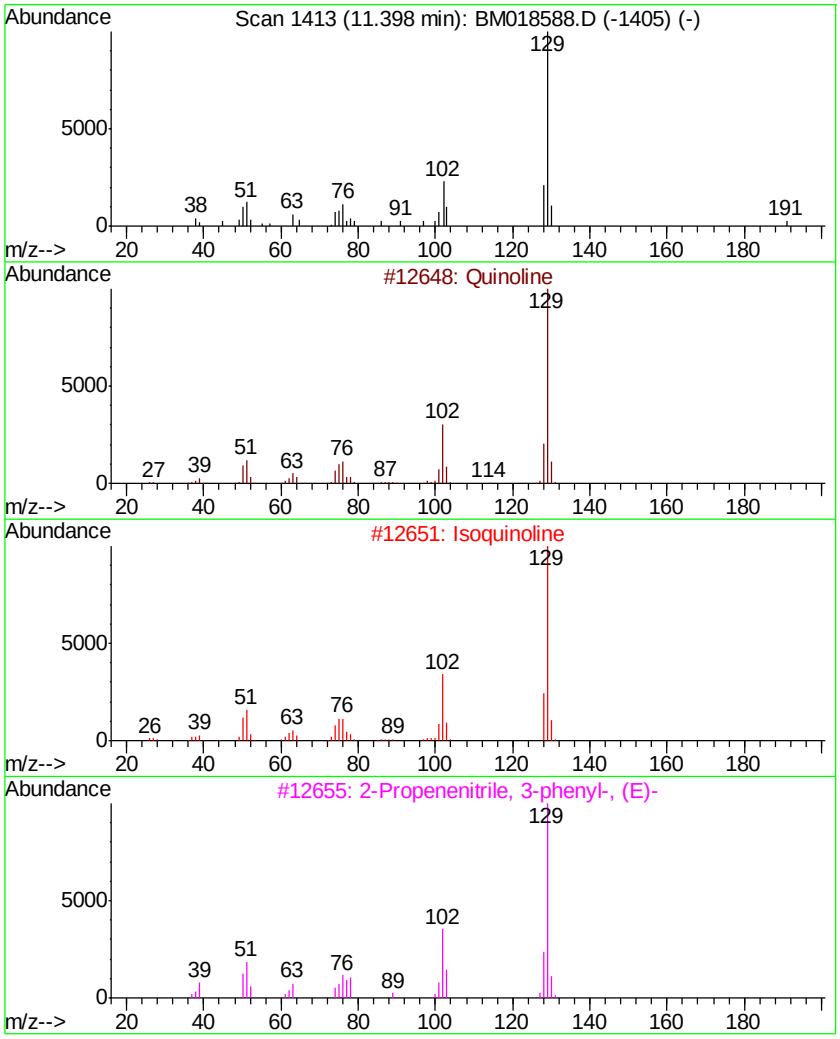
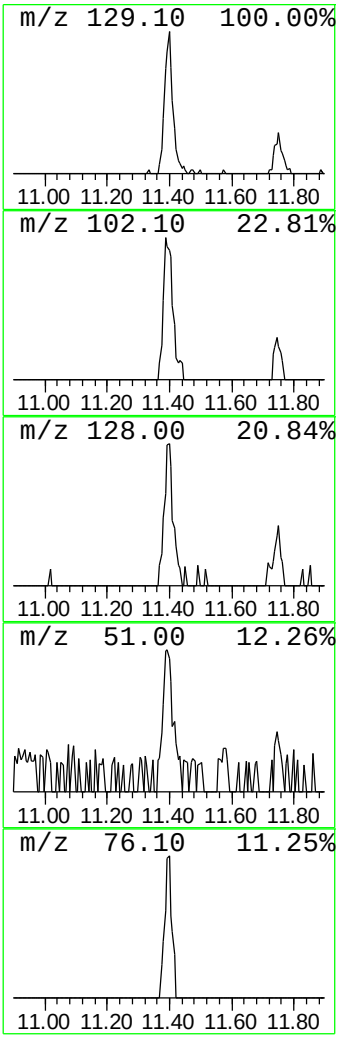
Peak Number 3 Quinoline Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.40	5.34 ng	73709	Naphthalene-d8	10.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Quinoline	129	C9H7N	000091-22-5	94
2	Isoquinoline	129	C9H7N	000119-65-3	91
3	2-Propenenitrile, 3-phenyl-, (E)-	129	C9H7N	001885-38-7	91
4	Benzeneacetonitrile, .alpha.-met...	129	C9H7N	000495-10-3	90
5	2-Quinolinecarboxylic acid	173	C10H7NO2	000093-10-7	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011619\
Data File : BM018588.D
Acq On : 16 Jan 2019 18:02
Operator : JU/SJ
Sample : K1149-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SW002-190114-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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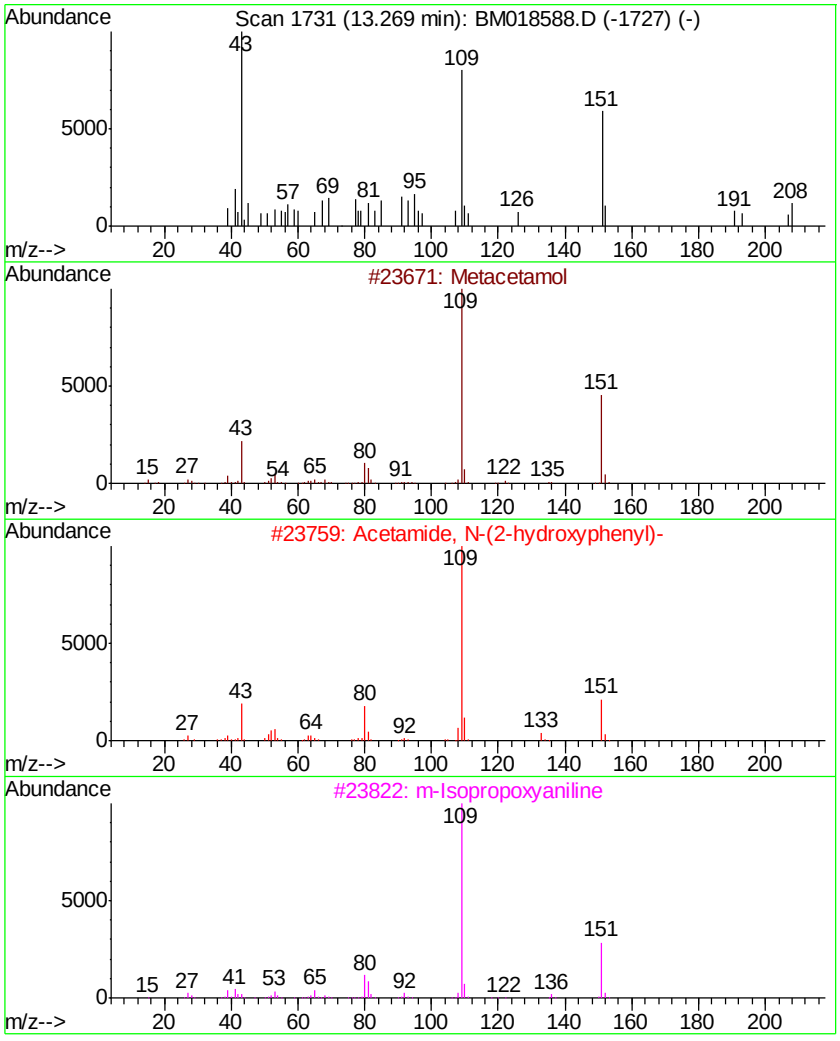
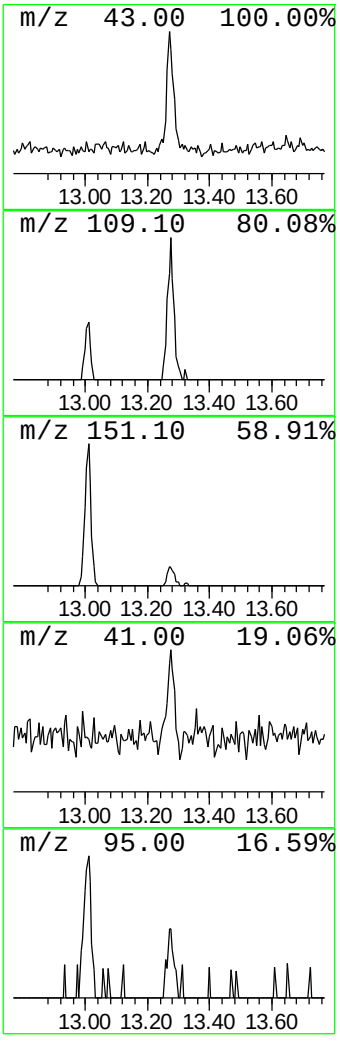
****

Peak Number 4 Metacetamol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.27	2.36 ng	44000	Acenaphthene-d10	14.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Metacetamol	151	C8H9NO2	000621-42-1	64
2	Acetamide, N-(2-hydroxyphenyl)-	151	C8H9NO2	000614-80-2	64
3	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	59
4	Diacetamate	193	C10H11NO3	002623-33-8	59
5	Acetaminophen	151	C8H9NO2	000103-90-2	59





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Data File : BM018588.D
Acq On : 16 Jan 2019 18:02
Operator : JU/SJ
Sample : K1149-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SW002-190114-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

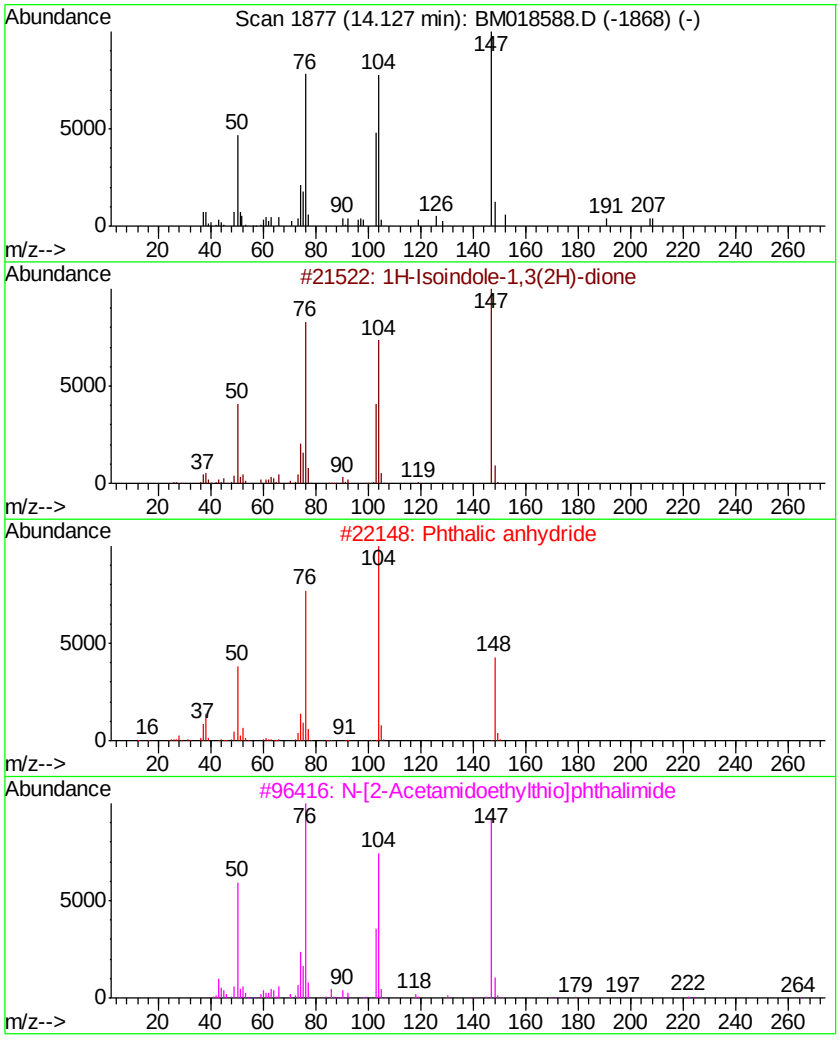
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

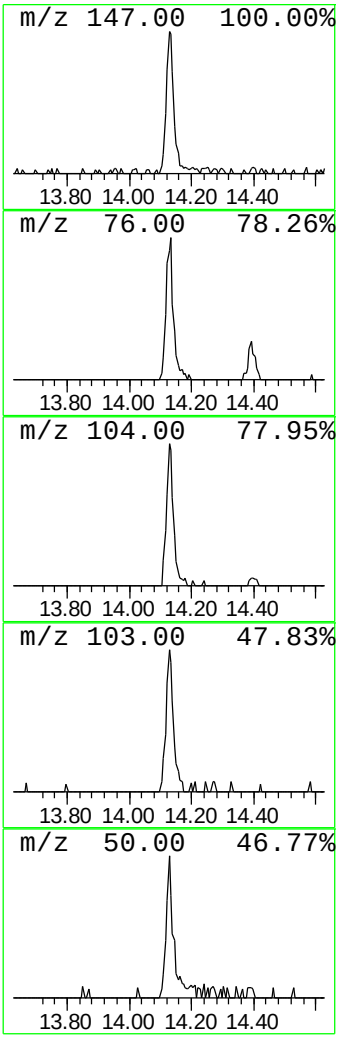
****

Peak Number 5 1H-Isoindole-1,3(2H)-dione Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.13	5.36 ng	100098	Acenaphthene-d10	14.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Isoindole-1,3(2H)-dione	147	C8H5NO2	000085-41-6	94
2	Phthalic anhydride	148	C8H4O3	000085-44-9	64
3	N-[2-Acetamidoethylthio]phthalimide	264	C12H12N2O3S	025158-14-9	64
4	Phthalic acid, monoethyl ester	194	C10H10O4	002306-33-4	64
5	2-Sulfobenzoic acid cyclic anhyd...	184	C7H4O4S	000081-08-3	64





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011619\
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Operator : JU/SJ
Sample : K1149-02
Misc :
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Instrument : BNA_M
ClientSampleId : SW002-190114-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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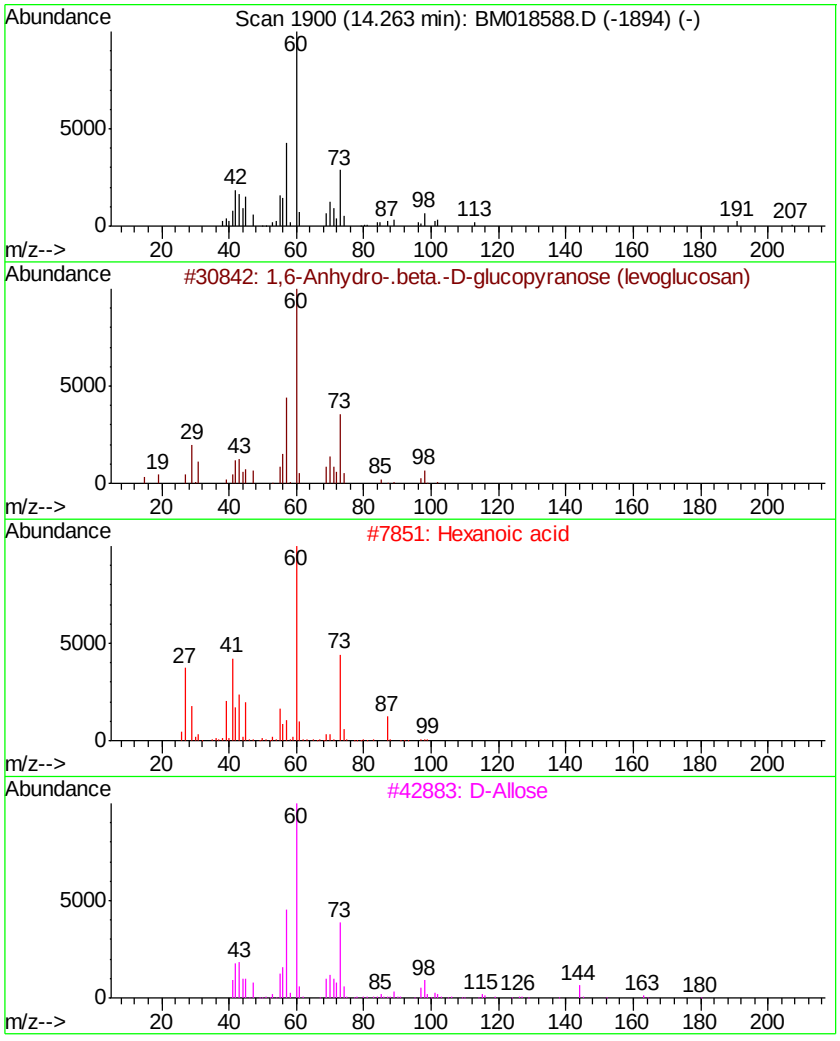
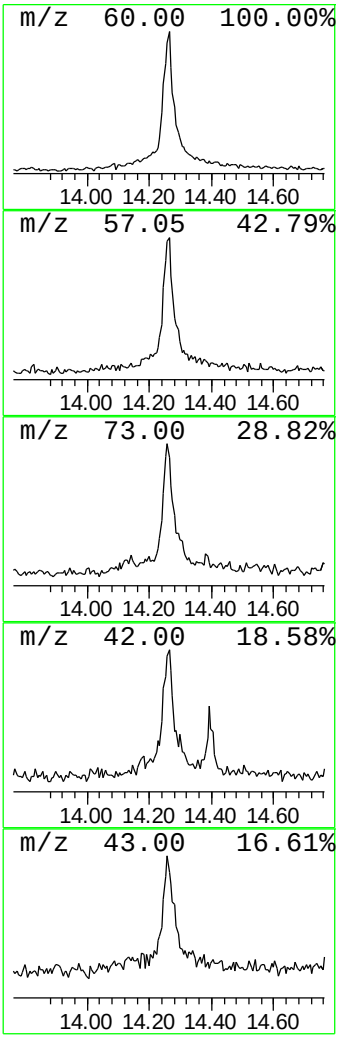
****

Peak Number 6 1,6-Anhydro-.beta.-D-glucop... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.26	9.58 ng	178749	Acenaphthene-d10	14.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6-Anhydro-.beta.-D-glucopyrano...	162	C6H10O5	000498-07-7	78
2	Hexanoic acid	116	C6H12O2	000142-62-1	64
3	D-Allose	180	C6H12O6	002595-97-3	58
4	Pentanoic acid	102	C5H10O2	000109-52-4	53
5	Heptanoic acid	130	C7H14O2	000111-14-8	50





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011619\
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Instrument : BNA_M
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

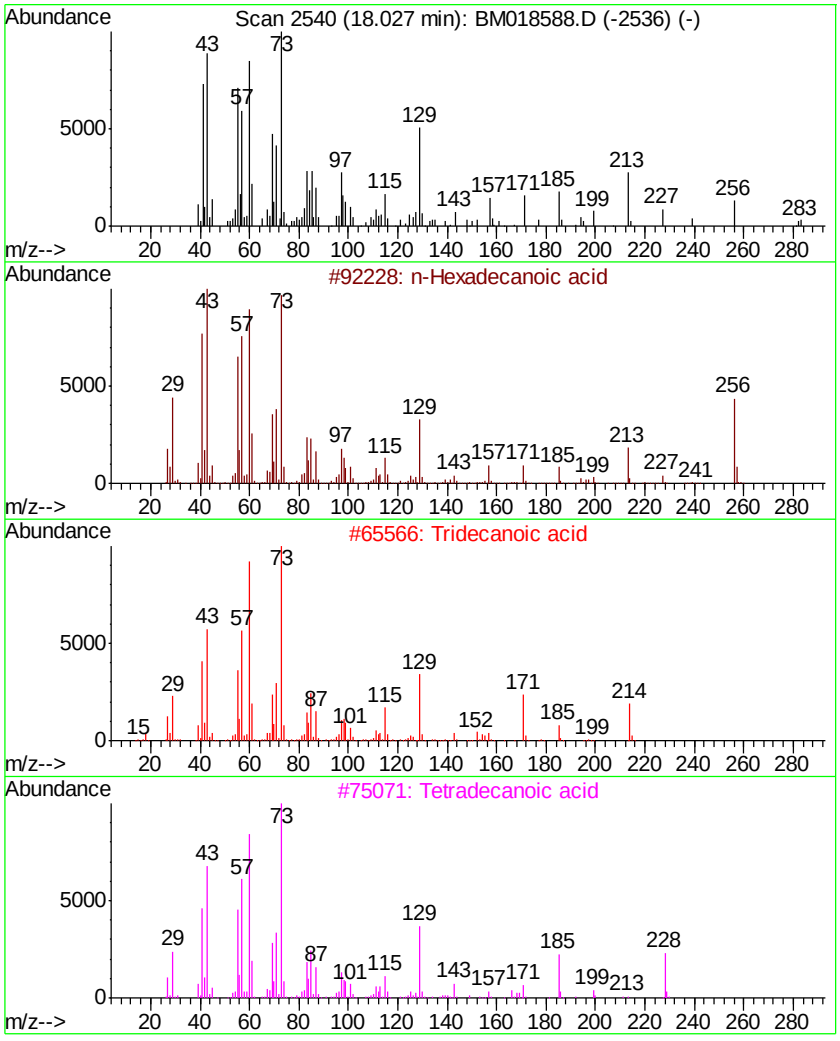
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

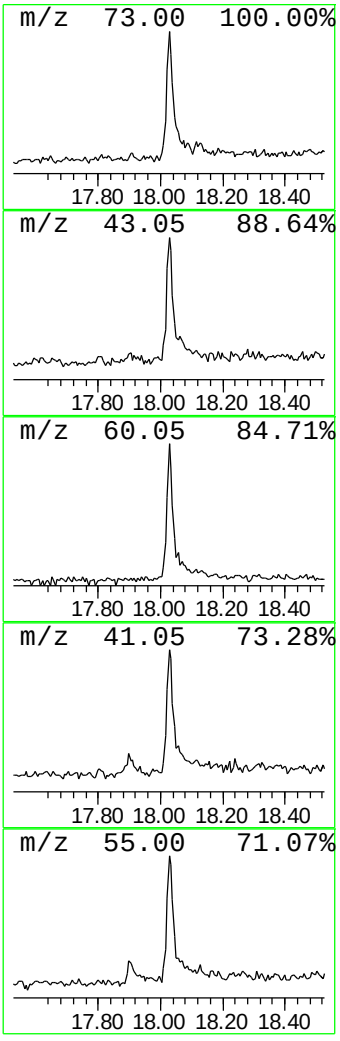
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.03	9.64 ng	235347	Phenanthrene-d10	17.14

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	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	35





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Instrument : BNA_M
ClientSampleId : SW002-190114-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

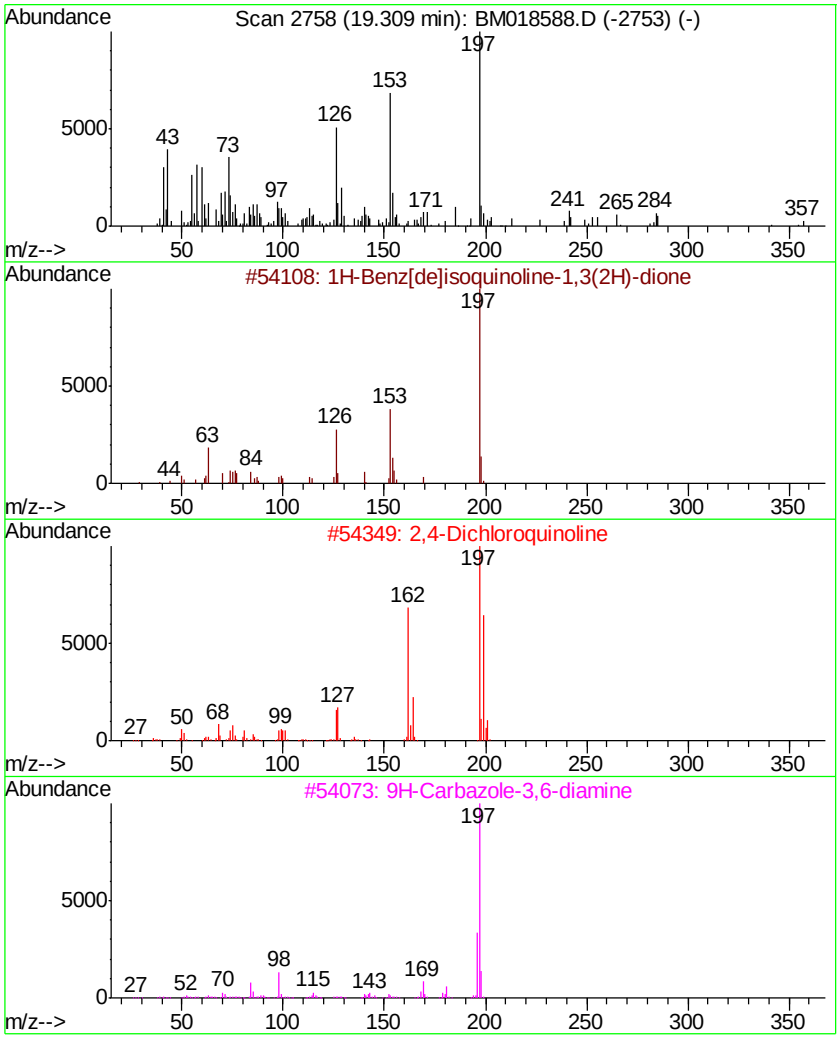
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

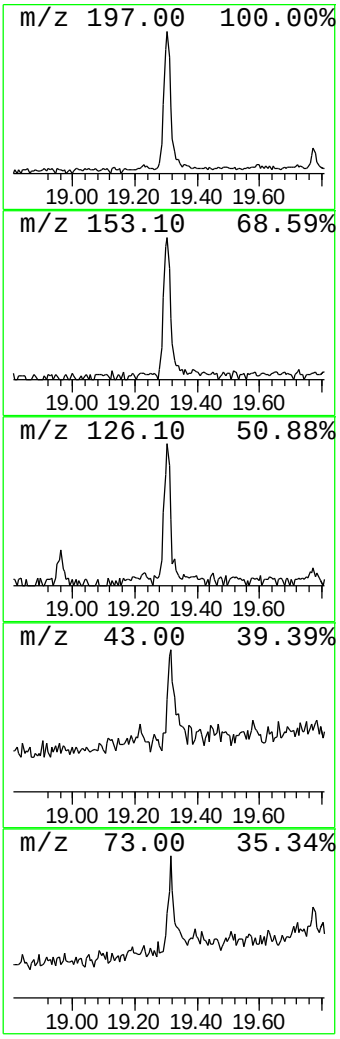
****

Peak Number 8 1H-Benz[de]isoquinoline-1,3... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.31	5.60 ng	218793	Chrysene-d12	21.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benz[de]isoquinoline-1,3(2H)-...	197	C12H7NO2	000081-83-4	83
2	2,4-Dichloroquinoline	197	C9H5Cl2N	000703-61-7	27
3	9H-Carbazole-3,6-diamine	197	C12H11N3	000086-71-5	25
4	1-Propanone, 2,2-dimethyl-1-(4-p...	254	C17H18O2	055814-54-5	22
5	Terephthalonitrile, 2-amino-3,5,...	197	C8H2F3N3	133622-66-9	22





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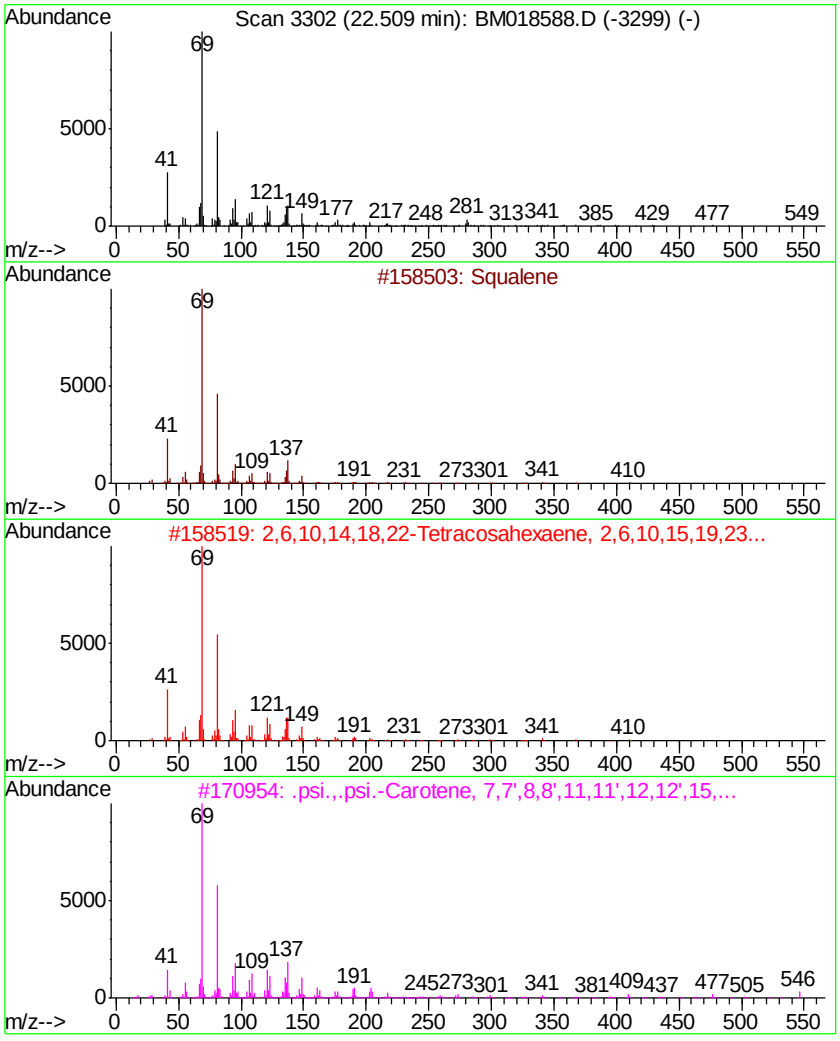
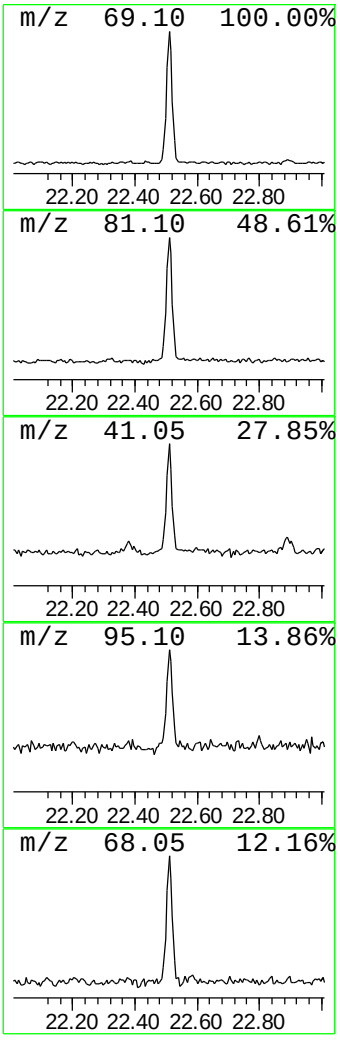
****

Peak Number 9 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.51	11.40 ng	380689	Perylene-d12	23.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	87
2	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	87
3	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	72
4	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	72
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64





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
unknown7.28	7.28	85.9	ng	875505	1	7.75	203890	20.0
Quinoline	11.40	5.3	ng	73709	2	10.54	275994	20.0
Metacetamol	13.27	2.4	ng	44000	3	14.39	373273	20.0
1H-Isoindole-1,3(...	14.13	5.4	ng	100098	3	14.39	373273	20.0
1,6-Anhydro-.beta...	14.26	9.6	ng	178749	3	14.39	373273	20.0
n-Hexadecanoic acid	18.03	9.6	ng	235347	4	17.14	488130	20.0
1H-Benz[de]isoqui...	19.31	5.6	ng	218793	5	21.33	781803	20.0
Squalene	22.51	11.4	ng	380689	6	23.61	668035	20.0