LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042221\
Data File : BM029599.D
Acq On : 22 Apr 2021 18:18
Operator : CG/JU
Sample : M2106-18
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SB-27-9.5-10.0

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-BM042121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029599.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.234	392	399	409	rBV	1302514	1884958	48.36%	9.122%
2	6.810	658	667	691	rBV	1201253	1995804	51.20%	9.658%
3	7.634	800	807	814	rBV	235184	375390	9.63%	1.817%
4	8.787	992	1003	1020	rBV	725458	1226657	31.47%	5.936%
5	10.410	1271	1279	1286	rBV	279824	471795	12.10%	2.283%
6	12.892	1694	1701	1718	rBV	1982038	2879963	73.88%	13.937%
7	13.180	1743	1750	1759	rBV	364355	556837	14.28%	2.695%
8	13.739	1838	1845	1855	rBV	73345	107437	2.76%	0.520%
9	14.274	1930	1936	1945	rBV2	442628	650504	16.69%	3.148%
10	14.839	2020	2032	2034	rBV2	41714	90295	2.32%	0.437%
11	15.416	2124	2130	2138	rBV	357932	497157	12.75%	2.406%
12	15.768	2183	2190	2208	rBV	1593274	2265185	58.11%	10.962%
13	17.021	2397	2403	2414	rBV	503020	759963	19.50%	3.678%
14	17.339	2452	2457	2465	rBV2	87946	129259	3.32%	0.626%
15	17.933	2552	2558	2566	rBV	185842	305209	7.83%	1.477%
16	19.115	2755	2759	2761	rBV	109226	129510	3.32%	0.627%
17	19.139	2761	2763	2769	rVB2	81755	102359	2.63%	0.495%
18	19.209	2772	2775	2784	rVB4	45401	73350	1.88%	0.355%
19	19.651	2845	2850	2859	rBV	3125853	3898117	100.00%	18.864%
20	19.945	2896	2900	2903	rBV4	29319	40143	1.03%	0.194%
21	20.303	2957	2961	2966	rBV	58367	71311	1.83%	0.345%
22	20.933	3064	3068	3075	rBV	115822	152054	3.90%	0.736%
23	21.203	3109	3114	3120	rBV	717829	918627	23.57%	4.445%
24	21.368	3139	3142	3146	rBV2	47715	50532	1.30%	0.245%
25	23.392	3480	3486	3496	rVB2	576590	1032192	26.48%	4.995%

Sum of corrected areas: 20664608

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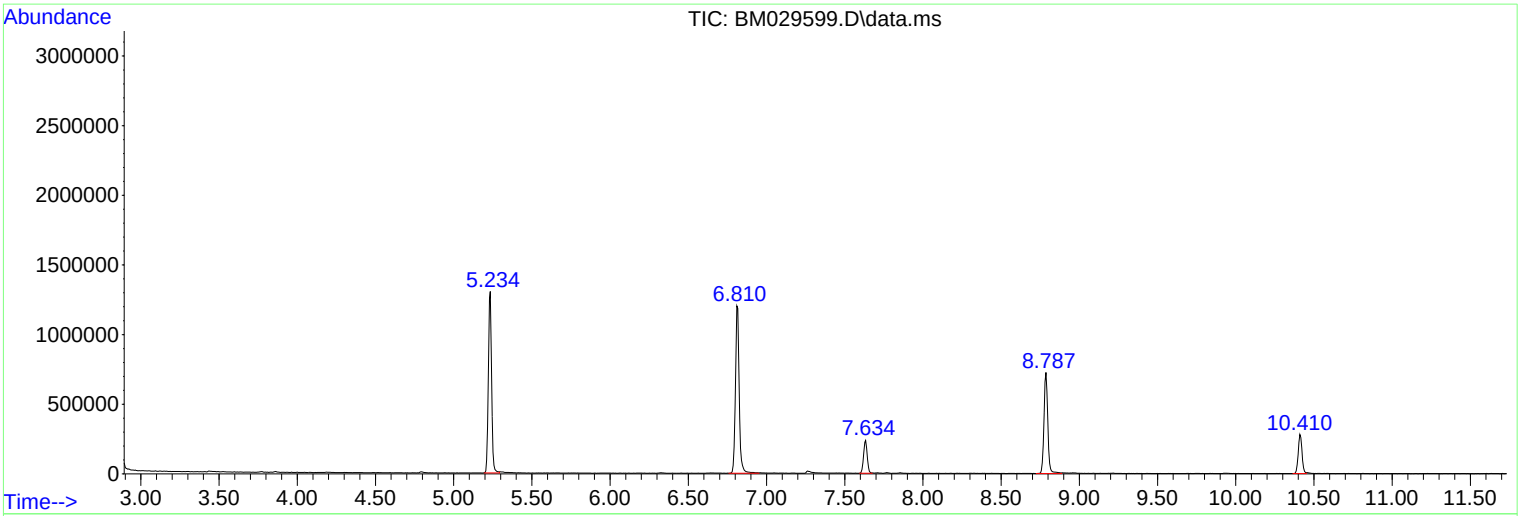
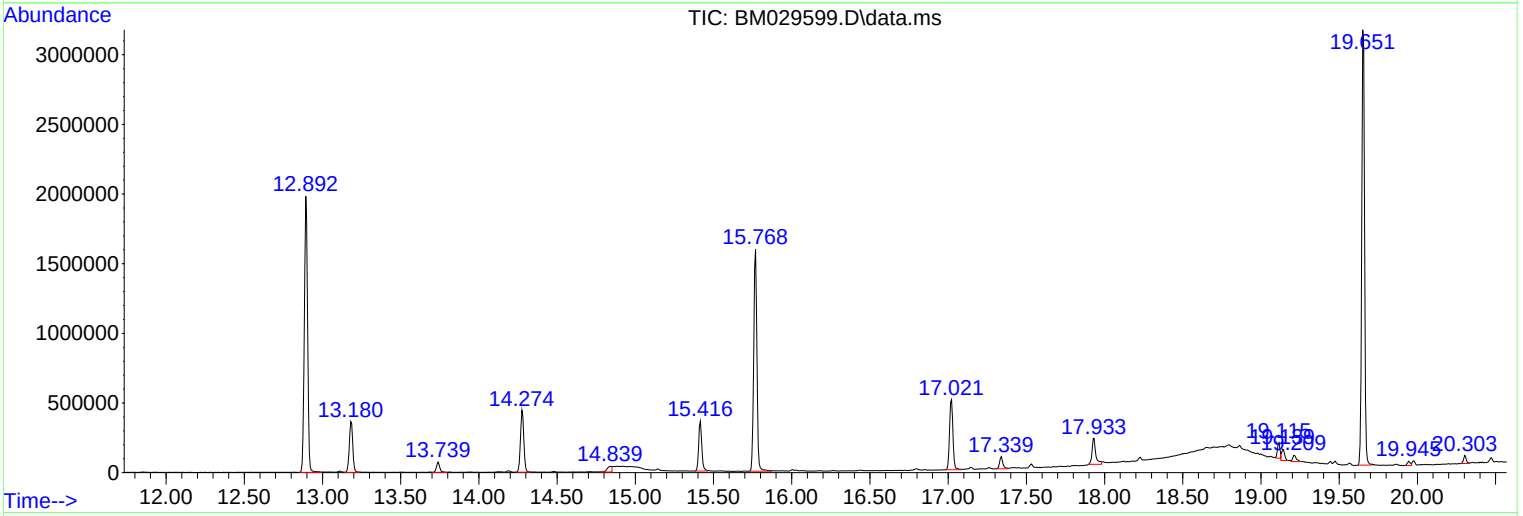
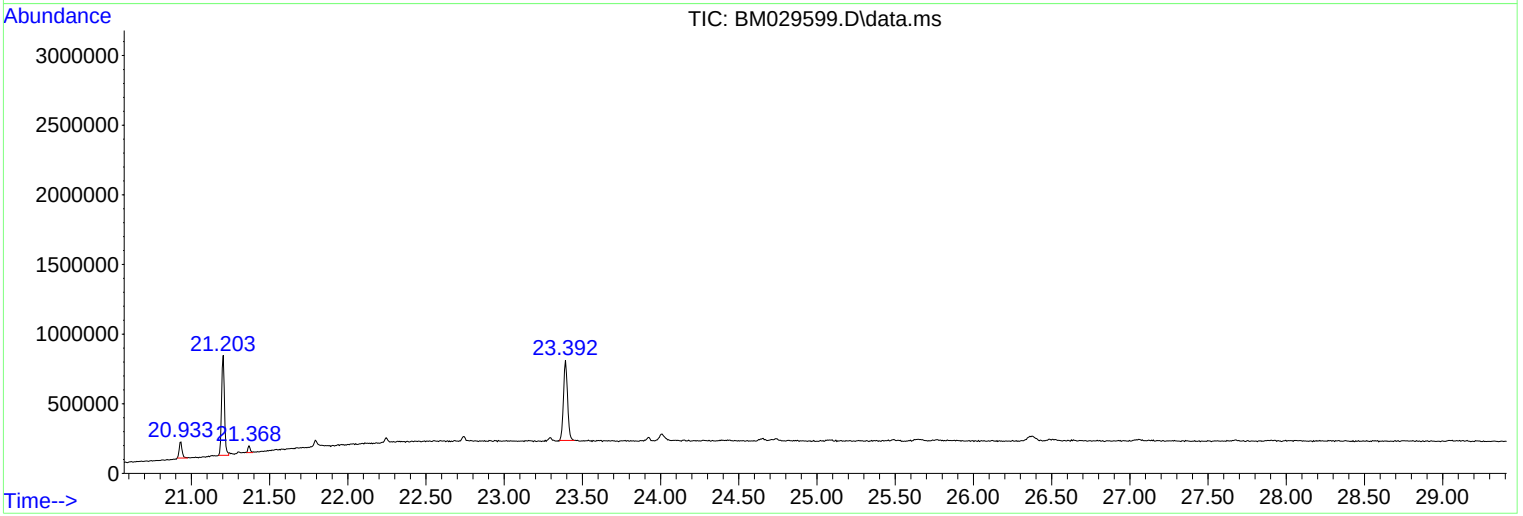
ClientSampleId :
SB-27-9.5-10.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P







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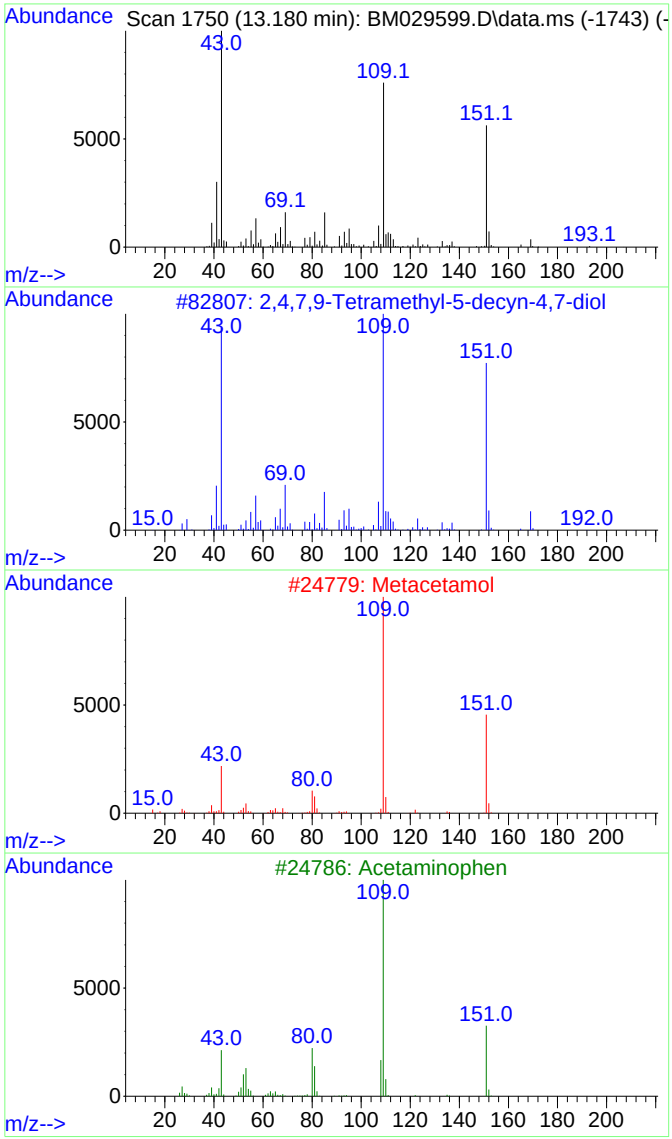
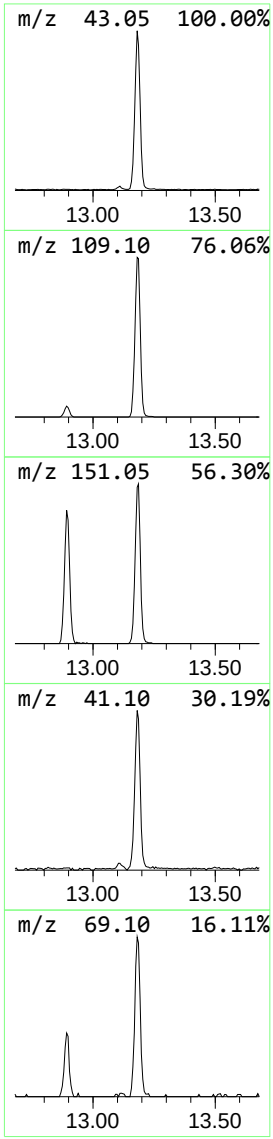
****
Peak Number 1 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.180	17.12 ng	556837	Acenaphthene-d10	14.275

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2	Metacetamol	151	C8H9NO2	000621-42-1	58
3	Acetaminophen	151	C8H9NO2	000103-90-2	58
4	p-Isopropoxyaniline	151	C9H13NO	007664-66-6	53
5	2-Propenal, 3-(2,2,6-trimethyl-7...	194	C12H18O2	055759-91-6	50





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Data File : BM029599.D
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Operator : CG/JU
Sample : M2106-18
Misc :
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Instrument :
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ClientSampleId :
SB-27-9.5-10.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042121.M
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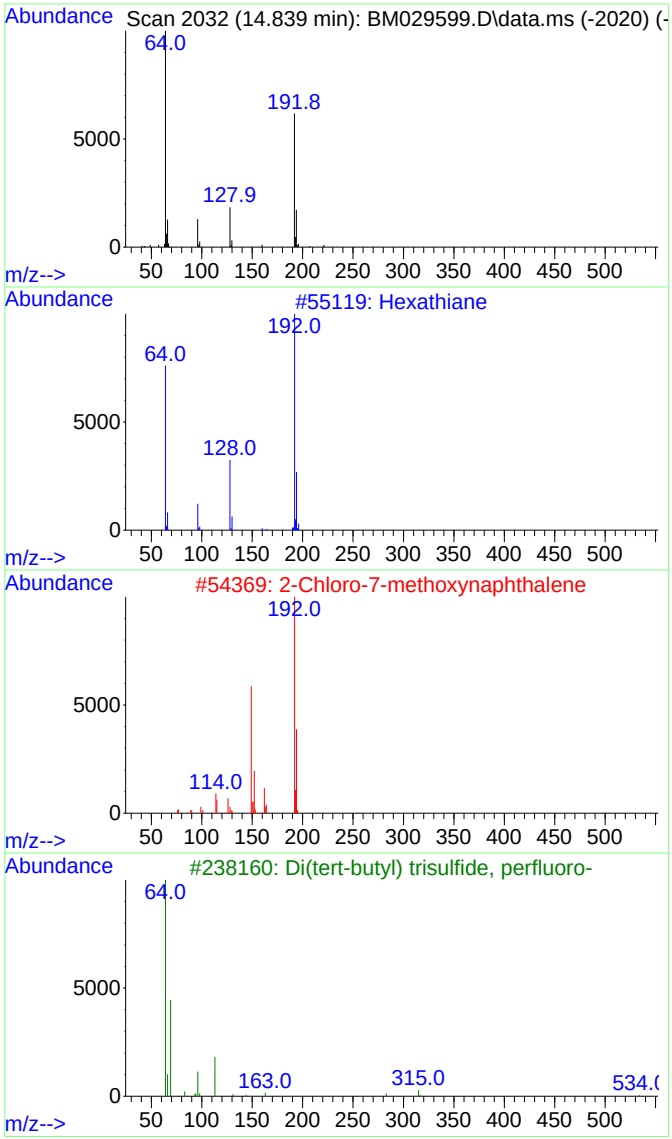
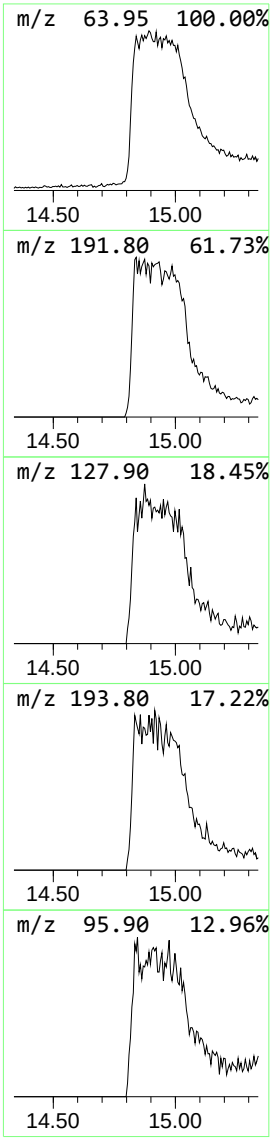
****

Peak Number 2 Hexathiane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.839	2.78 ng	90295	Acenaphthene-d10	14.275

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexathiane	192	S6	013798-23-7	91
2	2-Chloro-7-methoxynaphthalene	192	C11H9ClO	067061-67-0	42
3	Di(tert-butyl) trisulfide, perfl...	534	C8F18S3	016005-64-4	9
4	Ethyl Chloride	64	C2H5Cl	000075-00-3	4
5	Sulfur dioxide	64	O2S	007446-09-5	4





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Instrument : BNA_M
ClientSampleId : SB-27-9.5-10.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042121.M
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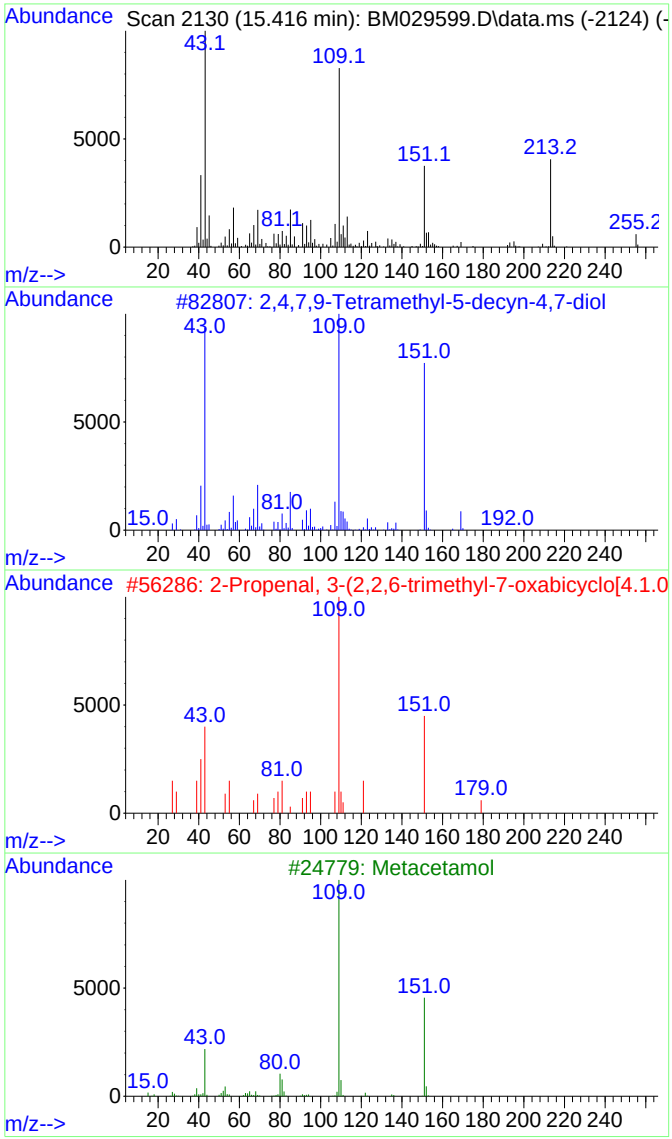
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

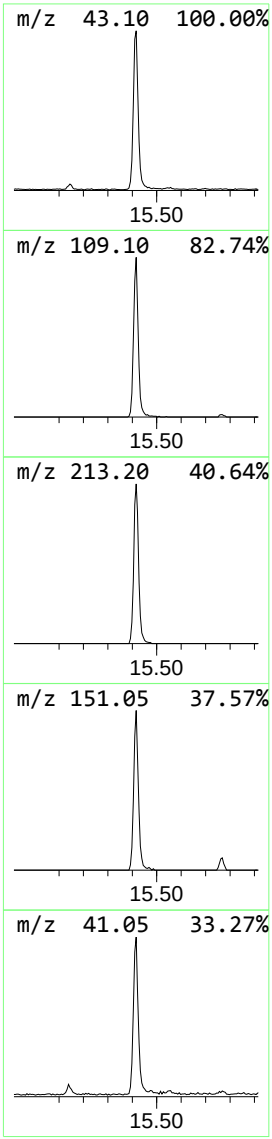
****

Peak Number 3 unknown15.146 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.416	15.29 ng	497157	Acenaphthene-d10	14.275

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	58
2	2-Propenal, 3-(2,2,6-trimethyl-7...	194	C12H18O2	055759-91-6	47
3	Metacetamol	151	C8H9NO2	000621-42-1	43
4	Acetaminophen	151	C8H9NO2	000103-90-2	43
5	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	38





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ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-27-9.5-10.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

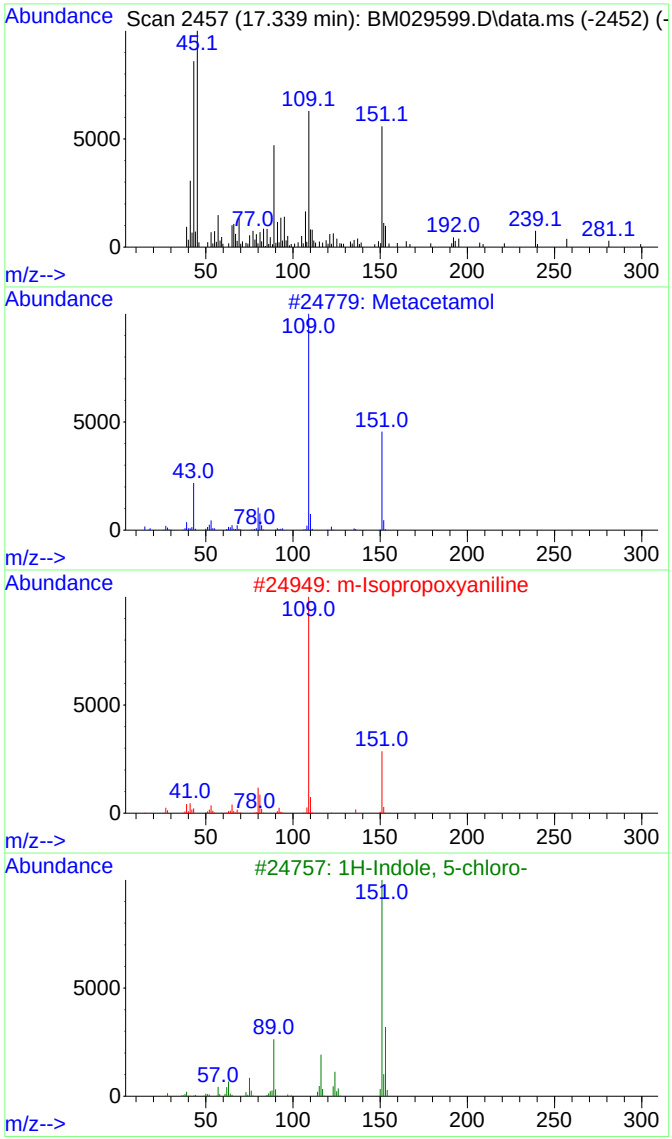
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

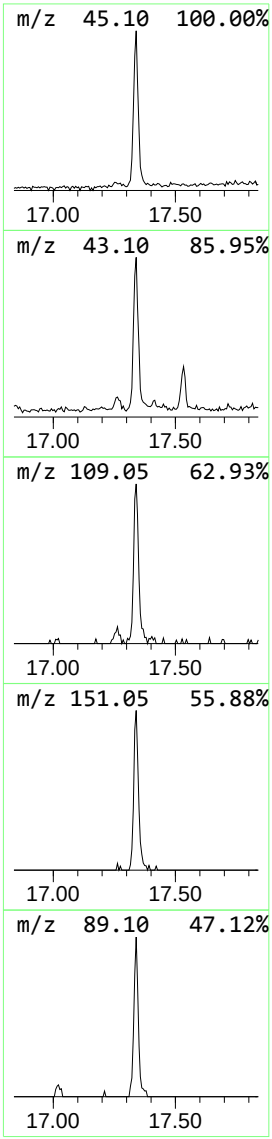
****

Peak Number 4 unknown17.339 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.339	3.40 ng	129259	Phenanthrene-d10	17.021

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Metacetamol	151	C8H9NO2	000621-42-1	25
2	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	25
3	1H-Indole, 5-chloro-	151	C8H6ClN	017422-32-1	22
4	1-Butene, 4-methoxy	86	C5H10O	004696-30-4	18
5	2-Decanol	158	C10H22O	001120-06-5	14





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ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SB-27-9.5-10.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

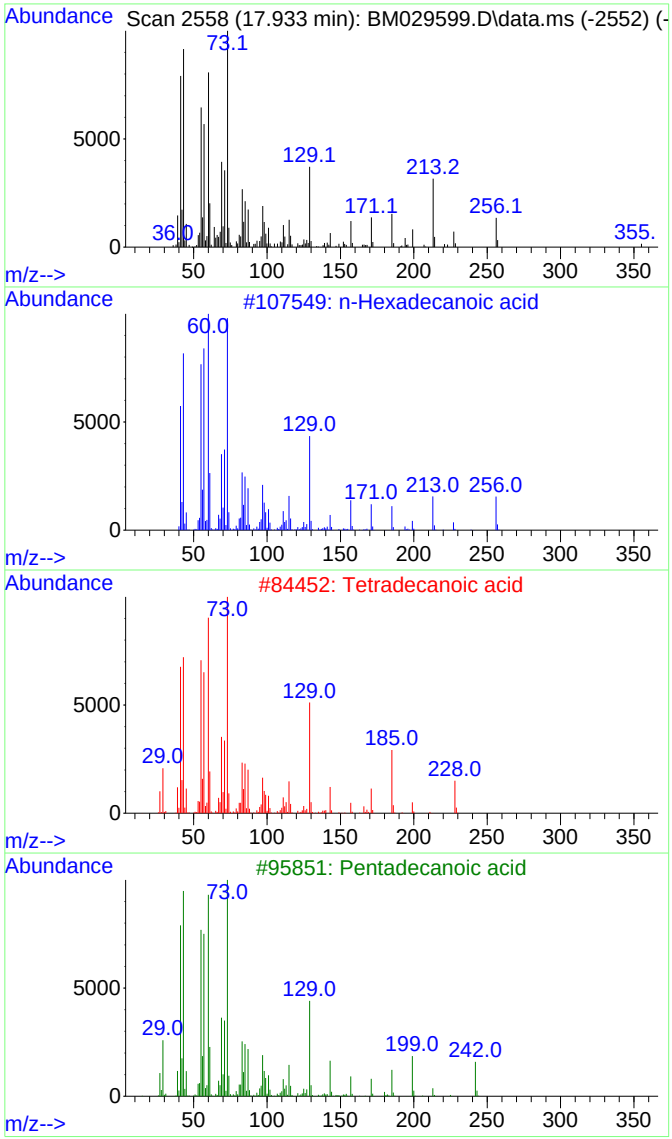
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

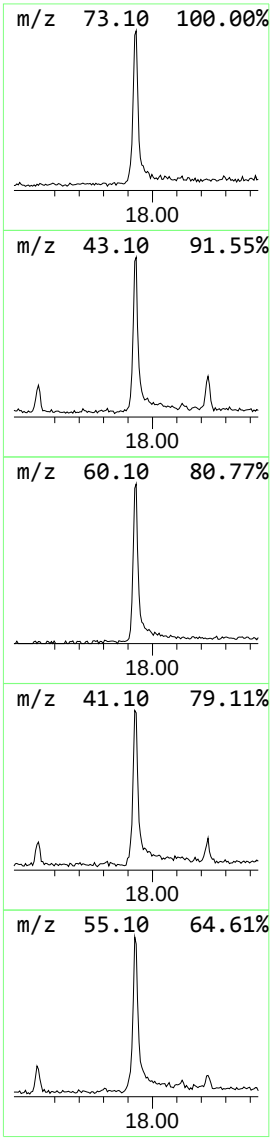
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.933	8.03 ng	305209	Phenanthrene-d10	17.021

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Octadecanoic acid	284	C18H36O2	000057-11-4	76
5	Tridecanoic acid	214	C13H26O2	000638-53-9	64





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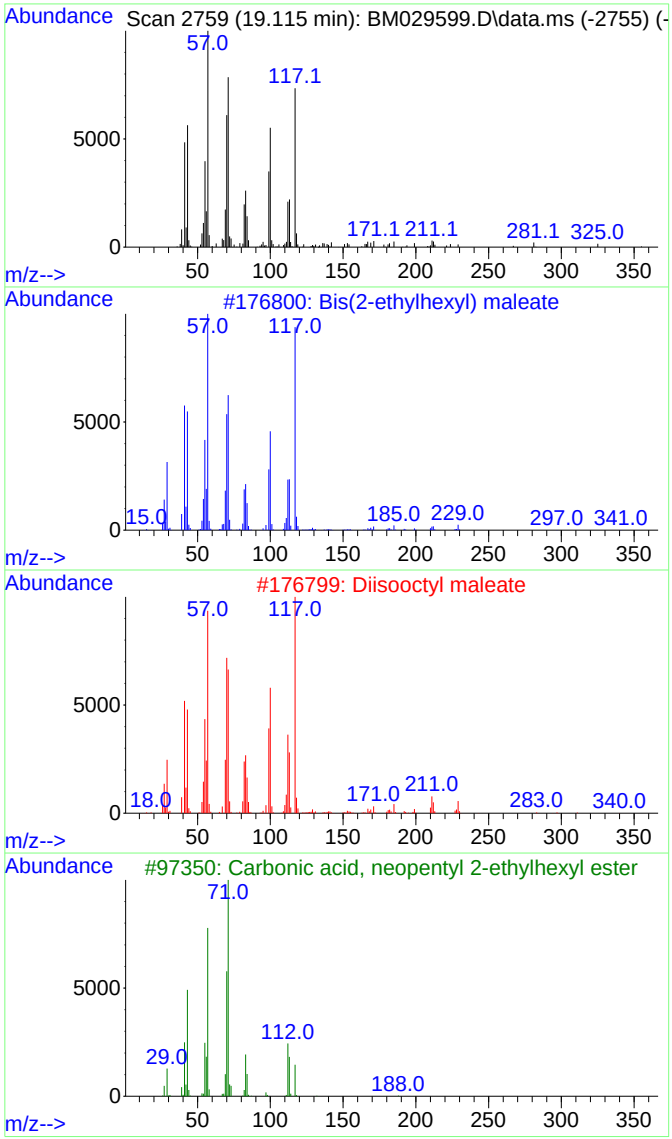
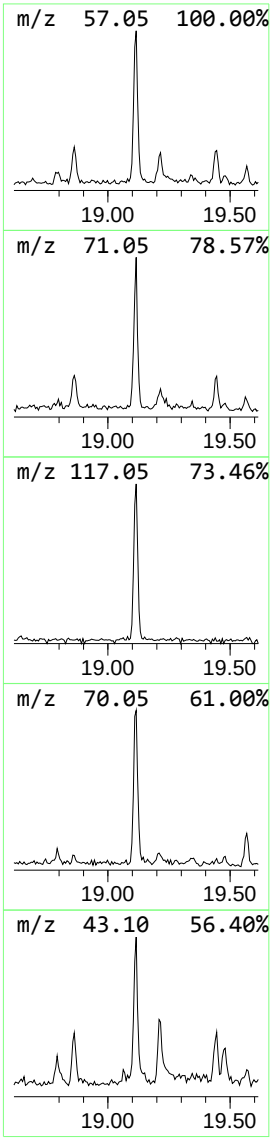
****

Peak Number 6 Bis(2-ethylhexyl) maleate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.115	2.82 ng	129510	Chrysene-d12	21.203

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bis(2-ethylhexyl) maleate	340	C20H36O4	000142-16-5	91
2	Diisooctyl maleate	340	C20H36O4	001330-76-3	50
3	Carbonic acid, neopentyl 2-ethyl...	244	C14H28O3	1000357-85-7	38
4	Fumaric acid, isopropyl nonyl ester	284	C16H28O4	1000339-29-5	35
5	Oxalic acid, bis(2-ethylhexyl) e...	314	C18H34O4	1000309-39-0	27





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Instrument : BNA_M
ClientSampleId : SB-27-9.5-10.0

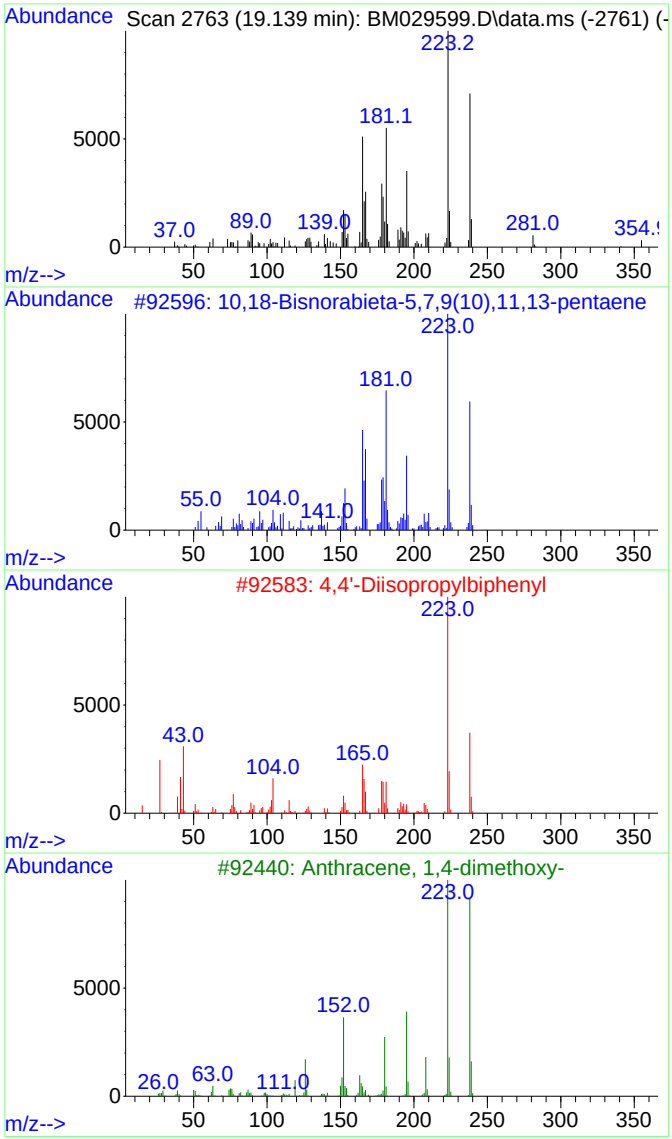
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

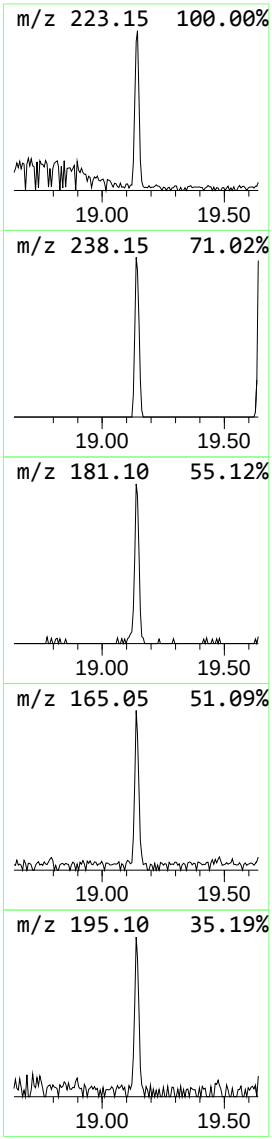
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 10,18-Bisnorabieta-5,7,9(10... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.139	2.23 ng	102359	Chrysene-d12	21.203

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10,18-Bisnorabieta-5,7,9(10),11,...	238	C18H22	006566-19-4	97
2	4,4'-Diisopropylbiphenyl	238	C18H22	018970-30-4	50
3	Anthracene, 1,4-dimethoxy-	238	C16H14O2	013076-29-4	43
4	9-Acridinecarboxylic acid	223	C14H9NO2	005336-90-3	43
5	2-Propenoic acid, 3-(3,4,5-trime...	238	C12H14O5	000090-50-6	41





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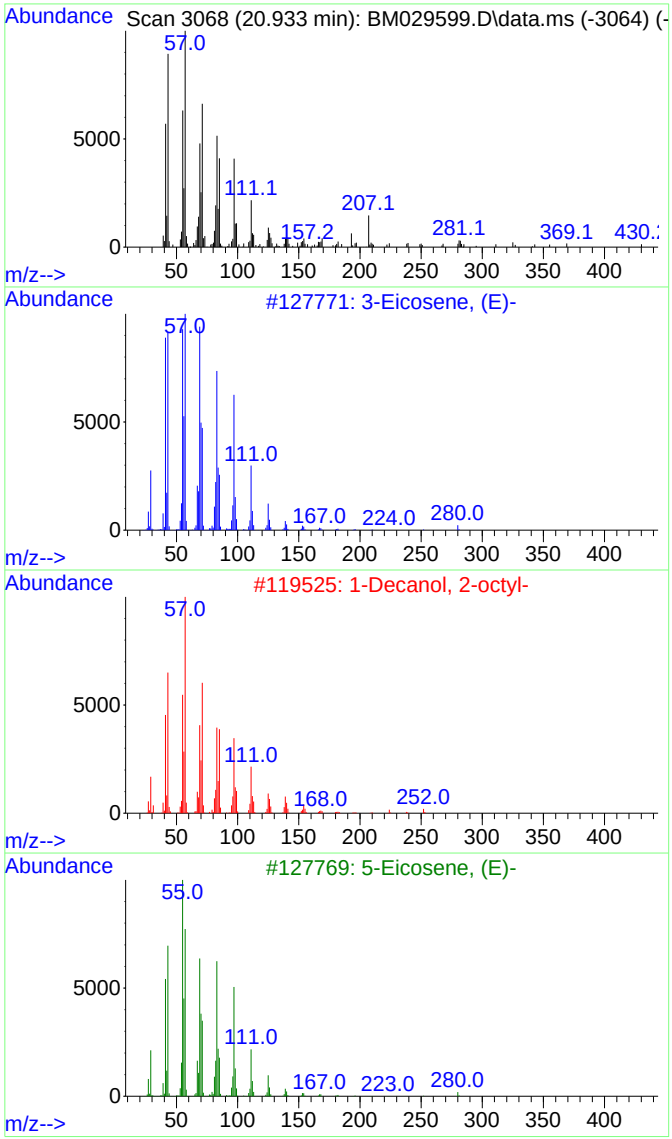
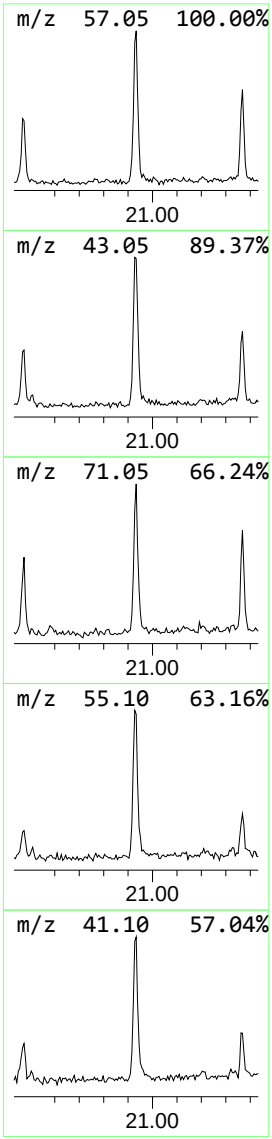
****
Peak Number 8 3-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.933	3.31 ng	152054	Chrysene-d12	21.203

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
2	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	87
3	5-Eicosene, (E)-	280	C20H40	074685-30-6	83
4	1-Eicosene	280	C20H40	003452-07-1	83
5	1-Heptadecene	238	C17H34	006765-39-5	78





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2,4,7,9-Tetrame...	13.180	17.1	ng	556837	3	14.275	650504	20.0
Hexathiane	14.839	2.8	ng	90295	3	14.275	650504	20.0
unknown15.146	15.416	15.3	ng	497157	3	14.275	650504	20.0
unknown17.339	17.339	3.4	ng	129259	4	17.021	759963	20.0
n-Hexadecanoic ...	17.933	8.0	ng	305209	4	17.021	759963	20.0
Bis(2-ethylhexy...	19.115	2.8	ng	129510	5	21.203	918627	20.0
10,18-Bisnorabi...	19.139	2.2	ng	102359	5	21.203	918627	20.0
3-Eicosene, (E)-	20.933	3.3	ng	152054	5	21.203	918627	20.0