LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060921\
Data File : BF124206.D
Acq On : 9 Jun 2021 13:25
Operator : JU/CG
Sample : PB136824BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB136824BL

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_F\METHODS\8270-BF060321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124206.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	5	10	15	rBV2	51715	66282	3.63%	0.626%
2	5.093	507	511	519	rBB	19544	25299	1.38%	0.239%
3	5.487	573	578	581	rBV	1478253	1323000	72.38%	12.490%
4	6.493	744	749	752	rBV	1280153	1289785	70.57%	12.177%
5	6.845	806	809	813	rBB	288504	239304	13.09%	2.259%
6	7.410	900	905	908	rBV	840690	882987	48.31%	8.336%
7	8.128	1023	1027	1031	rBV	380751	312144	17.08%	2.947%
8	9.210	1205	1211	1214	rBV	2110002	1735718	94.97%	16.387%
9	9.886	1322	1326	1329	rVB	481009	370777	20.29%	3.500%
10	10.681	1456	1461	1464	rBV	1357079	1225519	67.05%	11.570%
11	11.375	1575	1579	1582	rBV	426669	392770	21.49%	3.708%
12	12.963	1844	1849	1852	rBV	2013280	1827737	100.00%	17.256%
13	13.798	1984	1991	1995	rBV	23630	31076	1.70%	0.293%
14	13.845	1995	1999	2001	rVV	30021	38604	2.11%	0.364%
15	13.874	2001	2004	2008	rVB	83131	75161	4.11%	0.710%
16	14.010	2024	2027	2031	rVB	332911	288689	15.79%	2.725%
17	14.474	2104	2106	2110	rVB4	20682	20436	1.12%	0.193%
18	14.780	2154	2158	2162	rBV3	30455	35585	1.95%	0.336%
19	15.127	2212	2217	2221	rBV	27857	38985	2.13%	0.368%
20	15.486	2273	2278	2285	rVB2	177190	247160	13.52%	2.333%
21	15.945	2350	2356	2361	rVB5	18982	33787	1.85%	0.319%
22	16.445	2436	2441	2447	rBV6	17879	38520	2.11%	0.364%
23	16.974	2526	2531	2537	rBV8	21014	52852	2.89%	0.499%

Sum of corrected areas: 10592177

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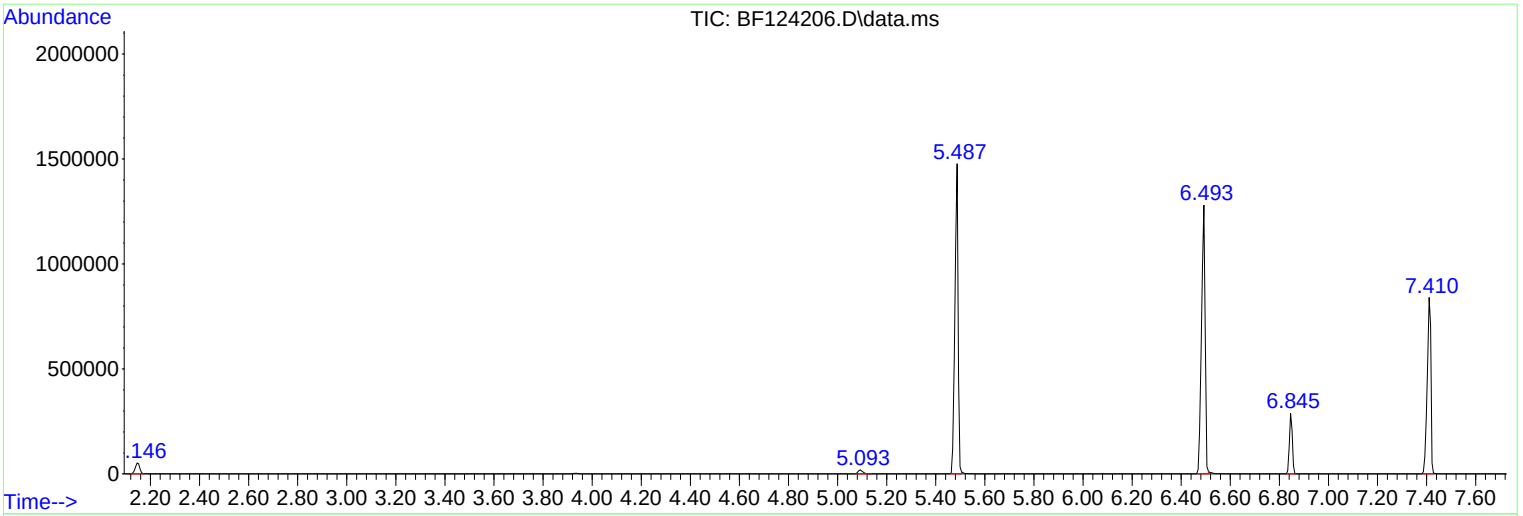
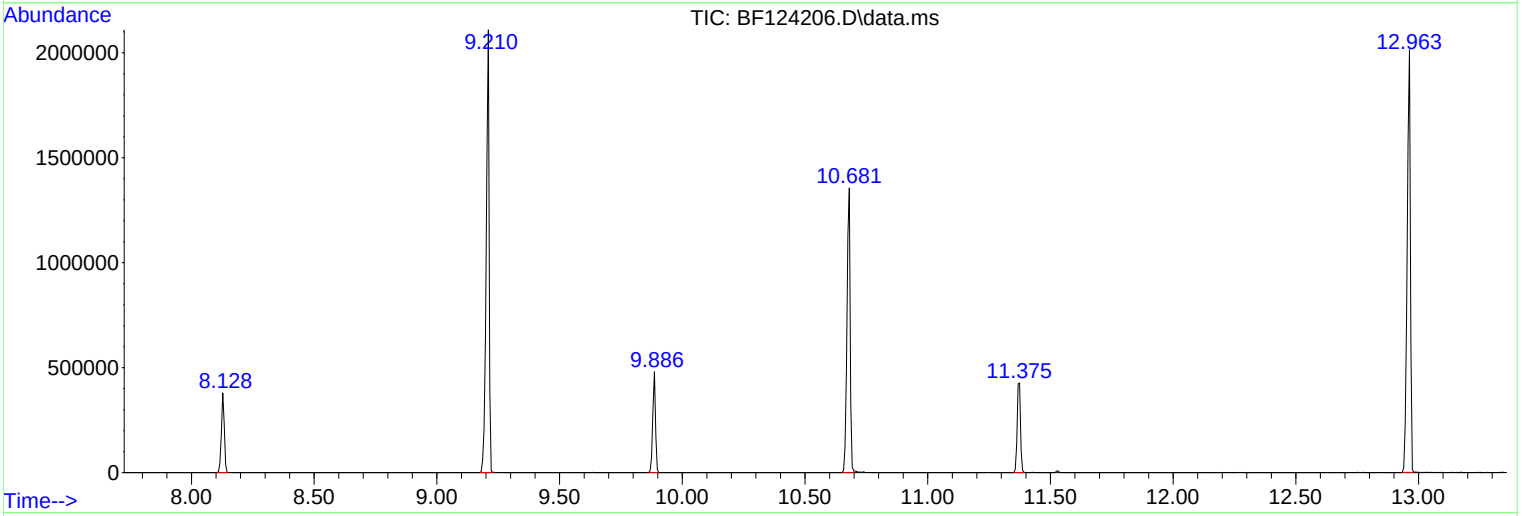
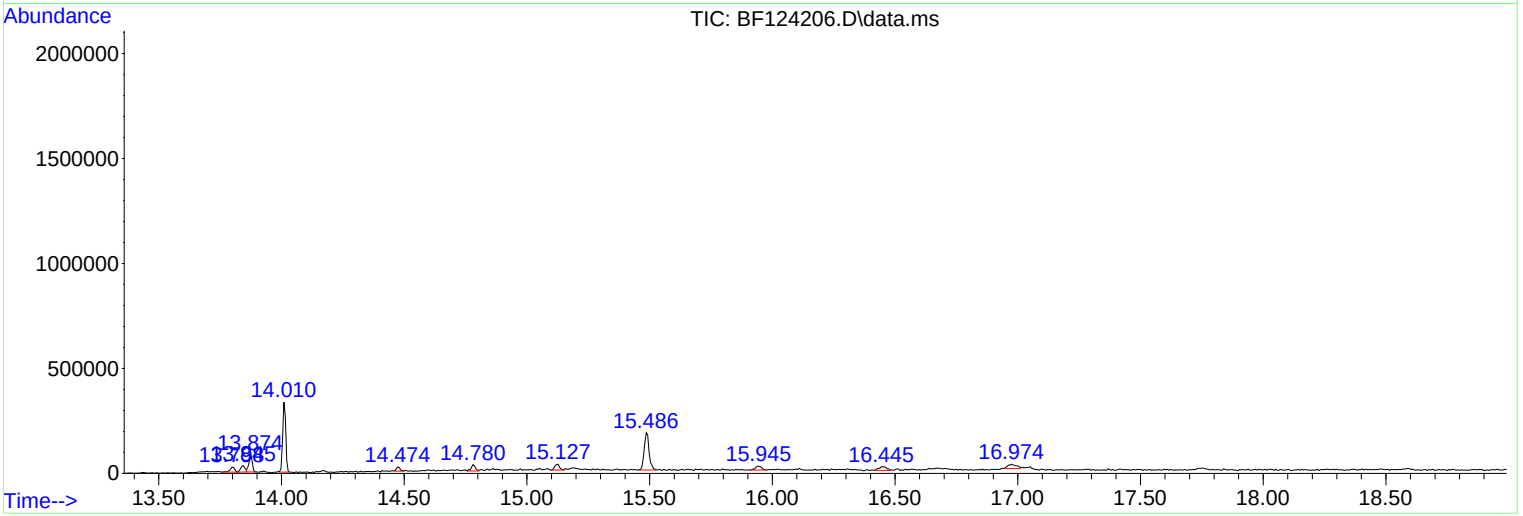
Instrument :
BNA_F
ClientSampleId :
PB136824BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.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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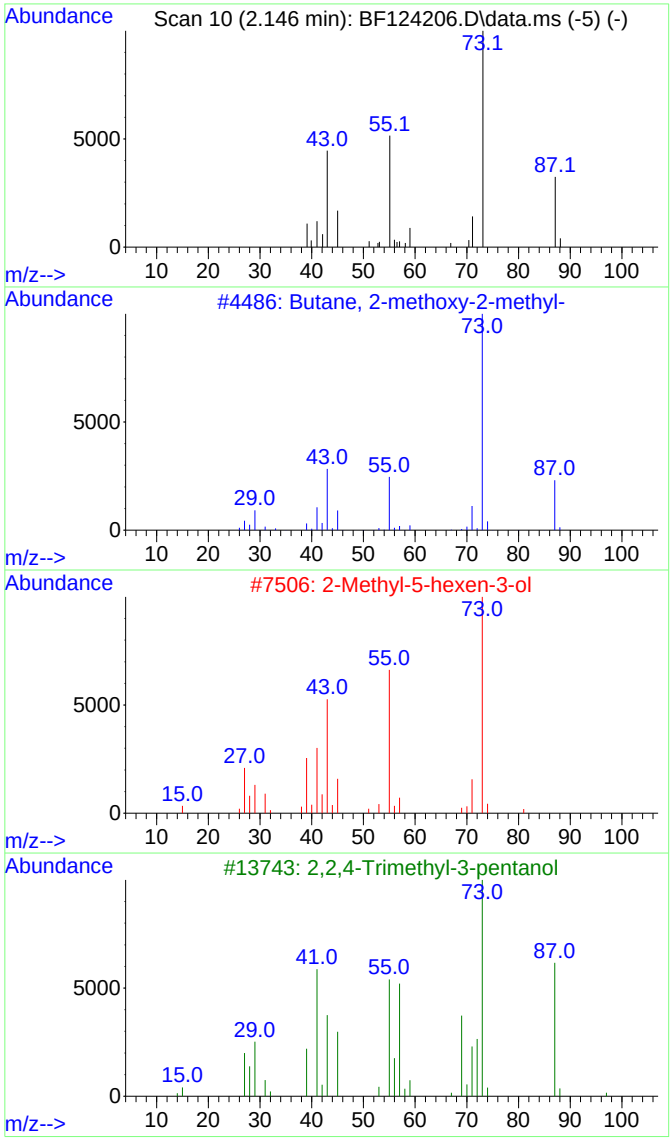
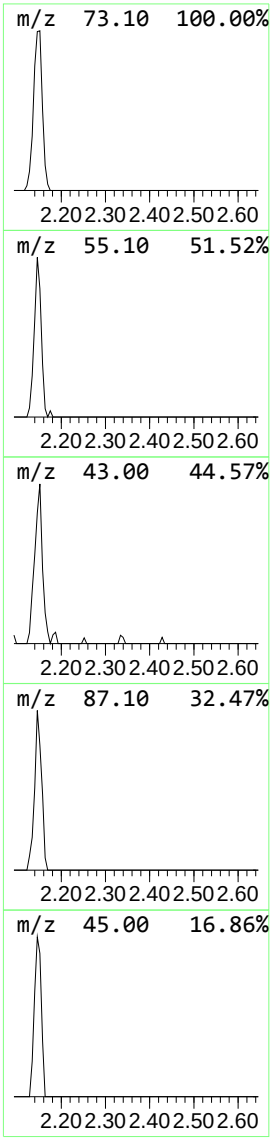
****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	5.54 ng	66282	1,4-Dichlorobenzene-d4	6.845

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	50
2	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	40
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	33
4	1-Pentanamine	87	C5H13N	000110-58-7	9
5	1,4-Butanediamine	88	C4H12N2	000110-60-1	9





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Operator : JU/CG
Sample : PB136824BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB136824BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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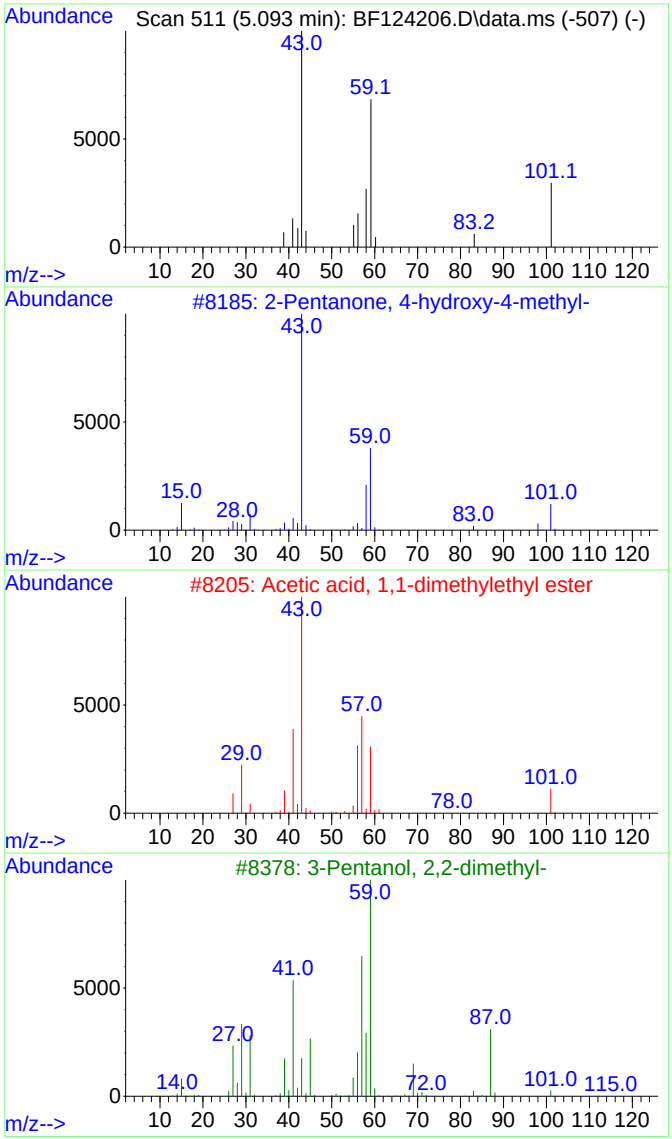
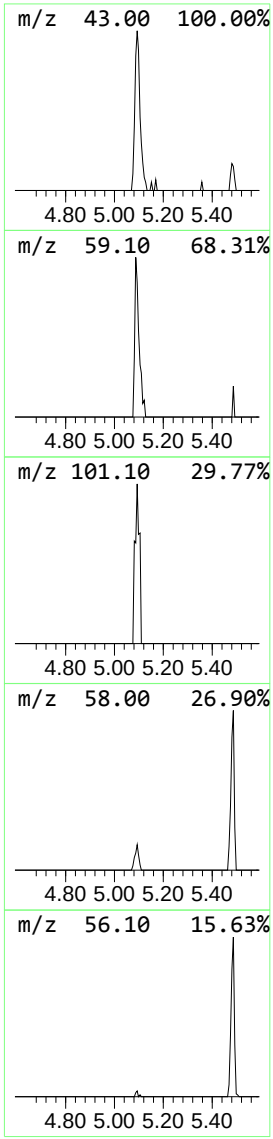
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	2.11 ng	25299	1,4-Dichlorobenzene-d4	6.845

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	43
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3	3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	28
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9
5	Oxetane, 2,2,4-trimethyl-	100	C6H12O	023120-44-7	9





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Sample : PB136824BL
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Instrument : BNA_F
ClientSampleId : PB136824BL

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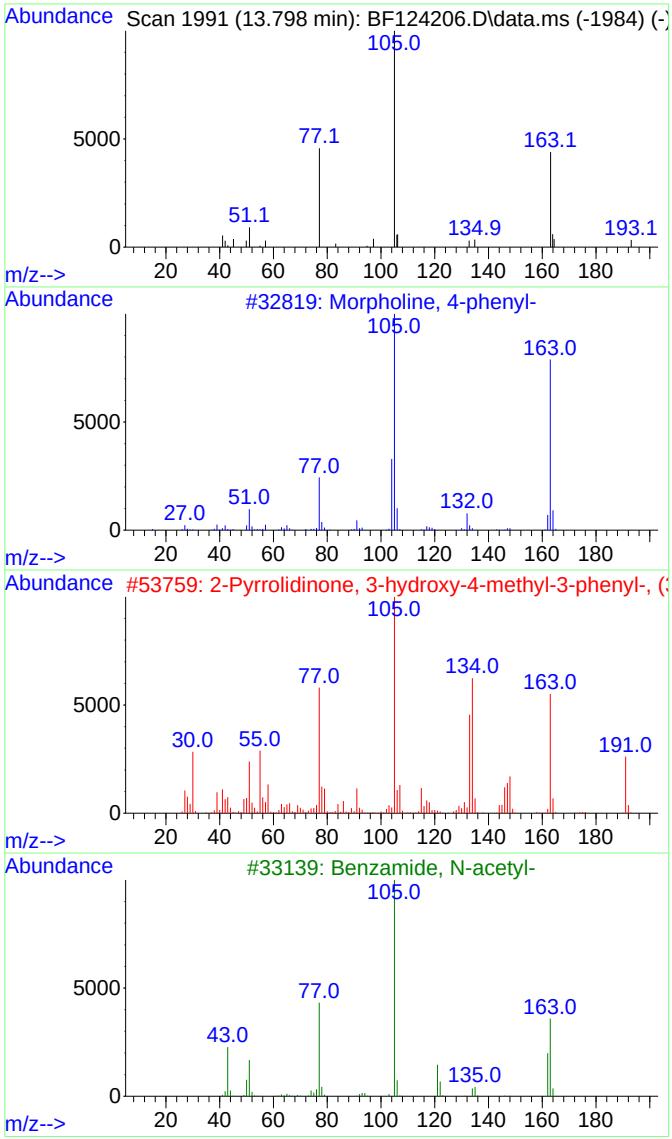
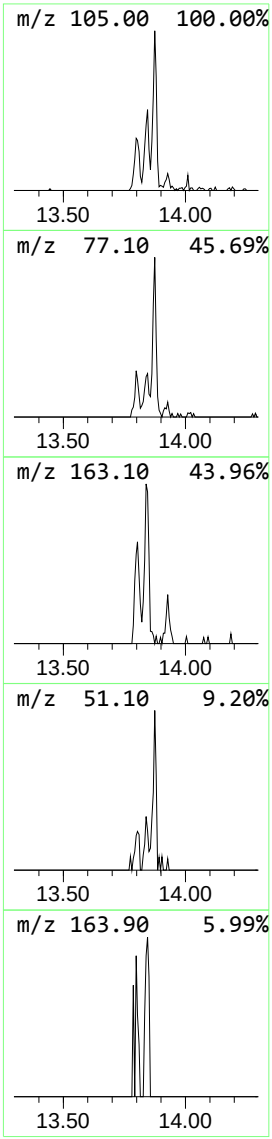
Peak Number 3 Morpholine, 4-phenyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.798	2.15 ng	31076	Chrysene-d12	14.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	56
2	2-Pyrrolidinone, 3-hydroxy-4-met...	191	C11H13NO2	104194-17-4	39
3	Benzamide, N-acetyl-	163	C9H9NO2	001575-95-7	39
4	3-(Benzoylthio)-2-methylpropanoi...	224	C11H12O3S	067714-34-5	37
5	Benzo[b]thiophene-3-carboxylic a...	343	C18H17NO4S	096334-43-9	37





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BNA_F
ClientSampleId :
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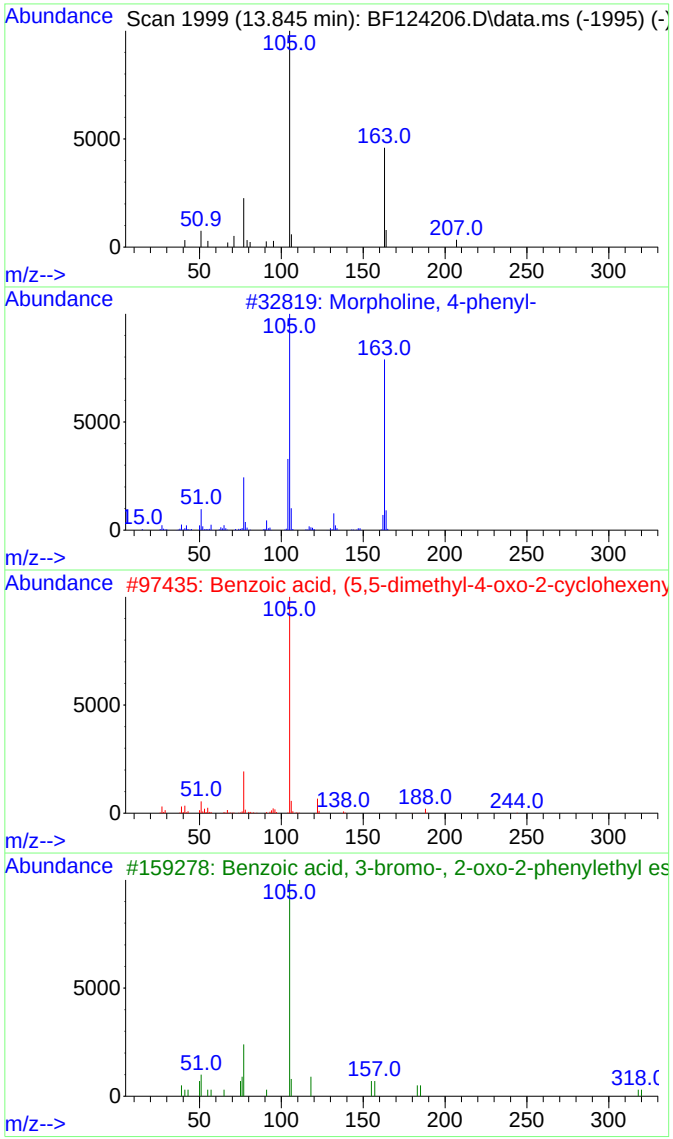
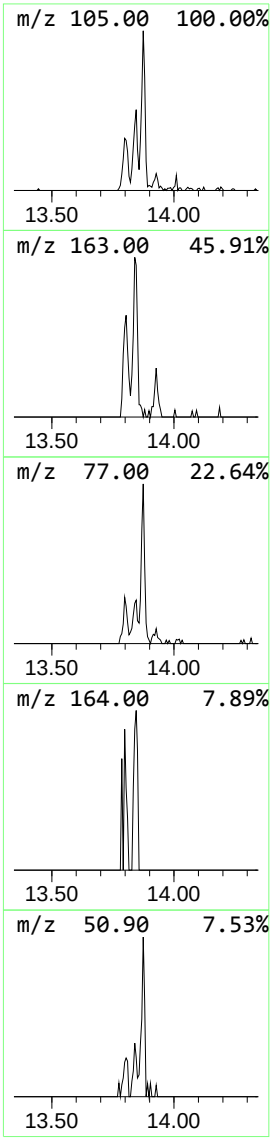
****

Peak Number 4 unknown13.845 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.845	2.67 ng	38604	Chrysene-d12	14.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	53
2	Benzoic acid, (5,5-dimethyl-4-ox...	244	C15H16O3	1000196-80-4	25
3	Benzoic acid, 3-bromo-, 2-oxo-2-...	318	C15H11BrO3	055153-27-0	17
4	Benzoic acid, 1-methylethyl ester	164	C10H12O2	000939-48-0	9
5	1,3-Dioxolane, 2,4-dimethyl-2-ph...	178	C11H14O2	004359-30-2	9





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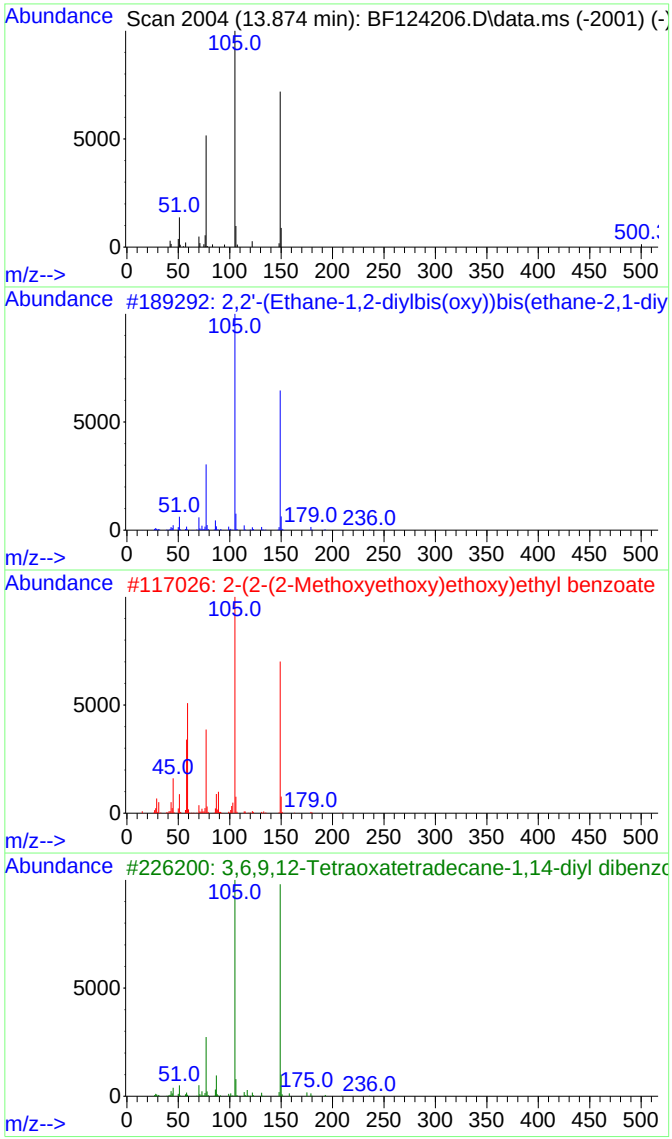
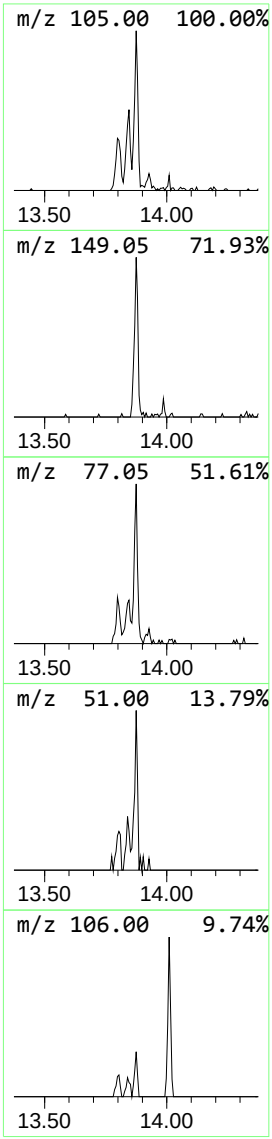
****
Peak Number 5 2,2'-(Ethane-1,2-diylbis(ox... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	5.21 ng	75161	Chrysene-d12	14.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	83
2	2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	78
3	3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	74
4	Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	72
5	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	64





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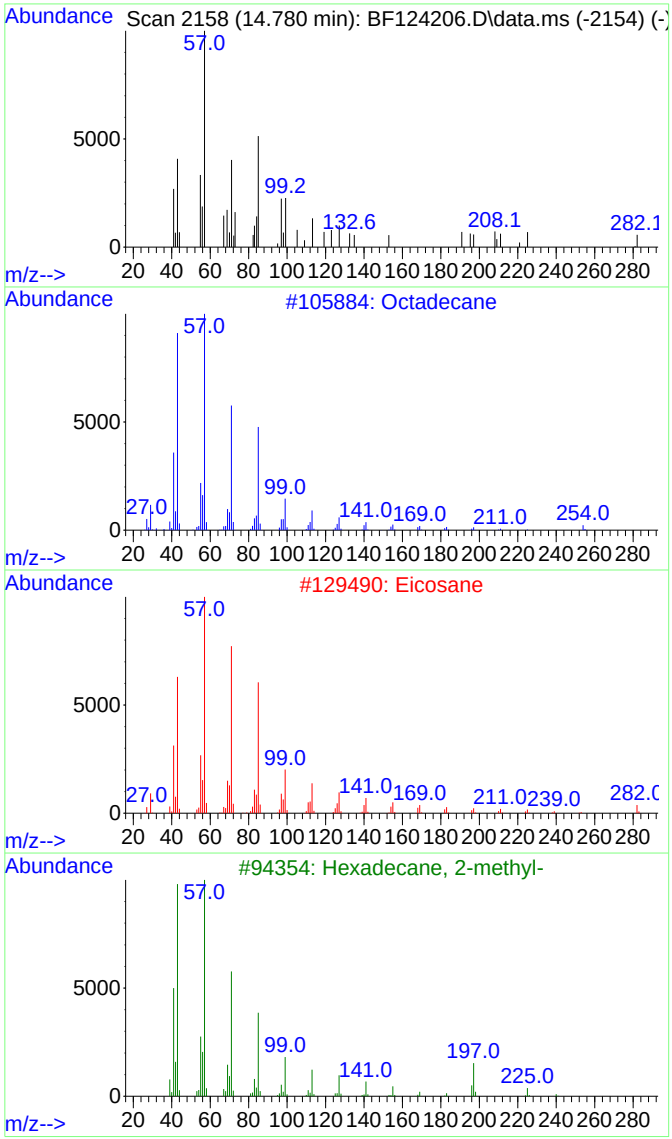
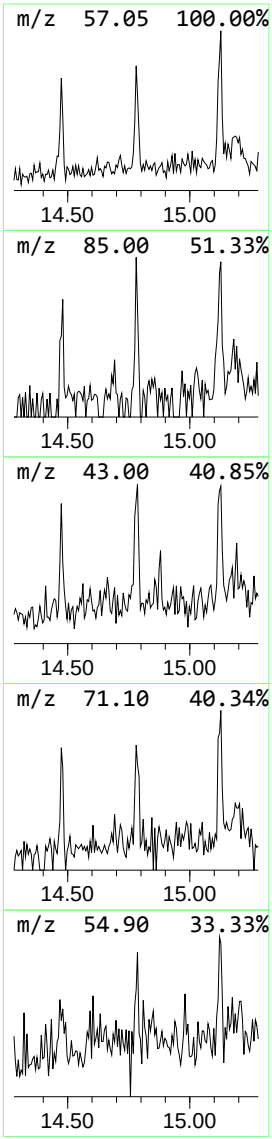
Peak Number 6 Octadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	2.88 ng	35585	Perylene-d12	15.486

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	53
2	Eicosane	282	C20H42	000112-95-8	49
3	Hexadecane, 2-methyl-	240	C17H36	001560-92-5	47
4	Octacosane	394	C28H58	000630-02-4	43
5	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	40





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TIC Library : C:\DATABASE\NIST11.L
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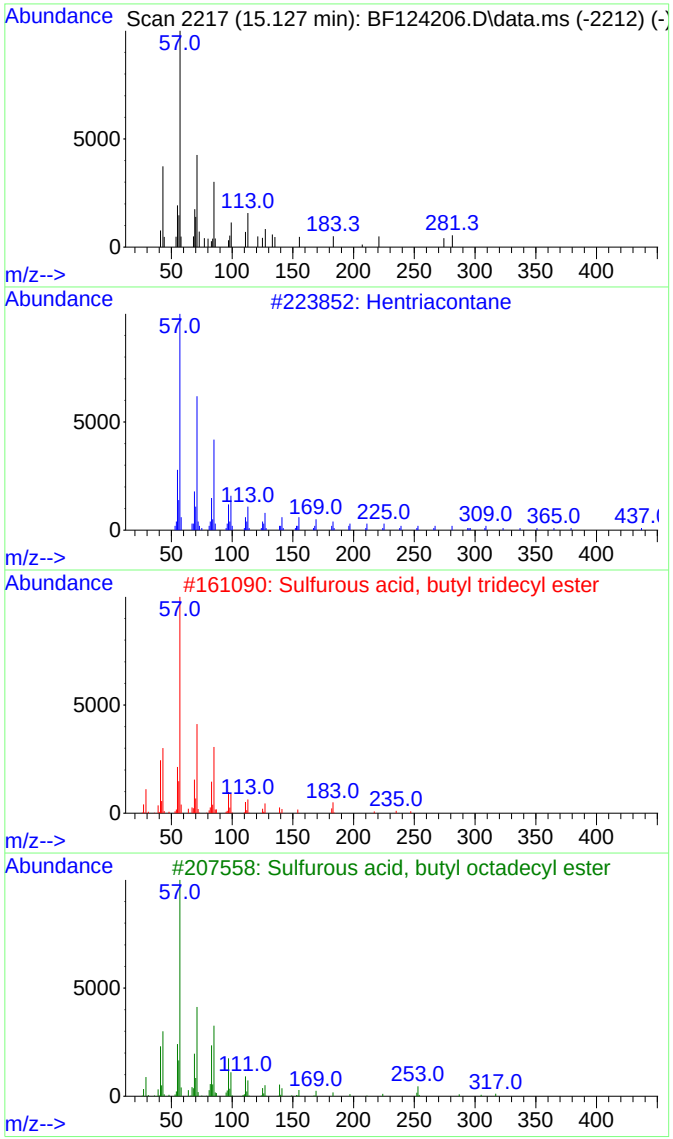
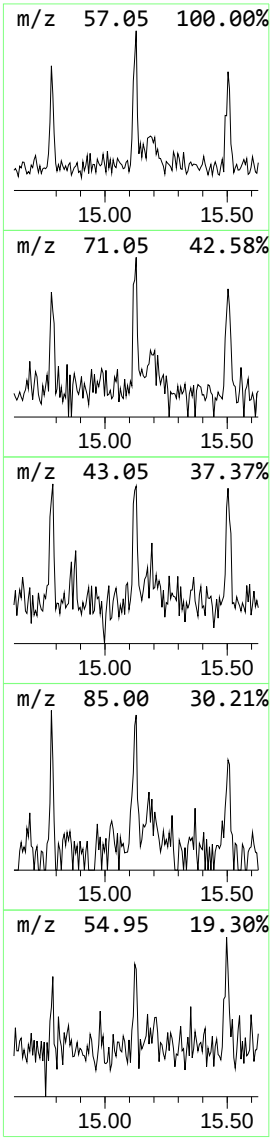
Peak Number 7 Hentriacontane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.127	3.15 ng	38985	Perylene-d12	15.486

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	86
2	Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	64
3	Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	64
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	59
5	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	59





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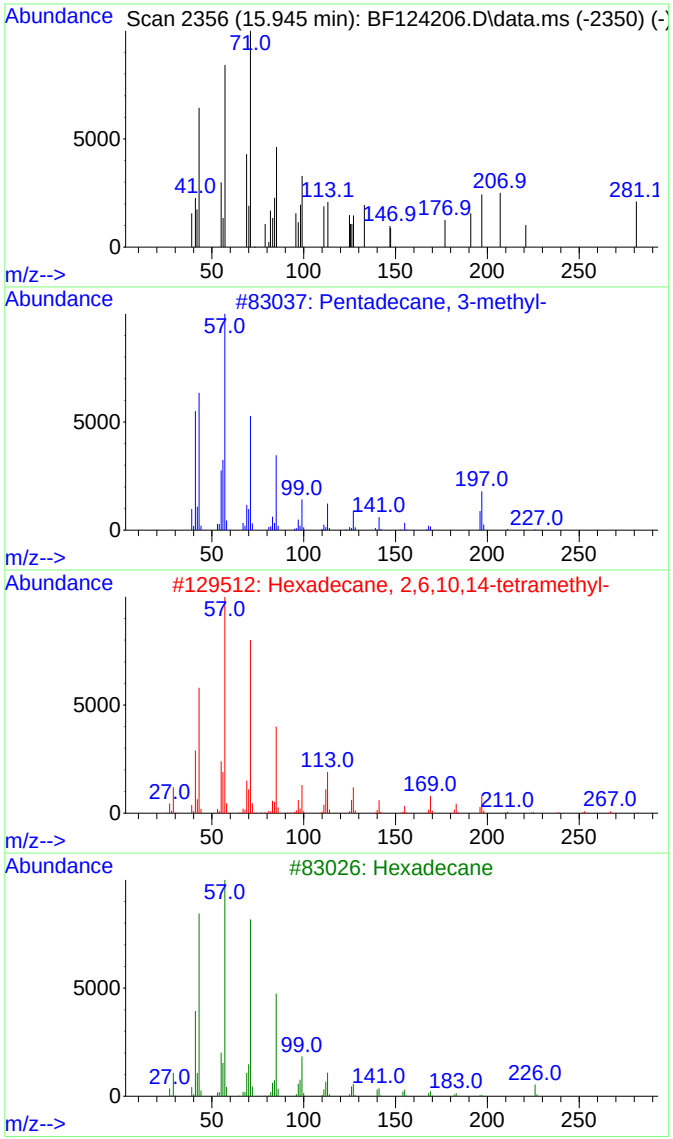
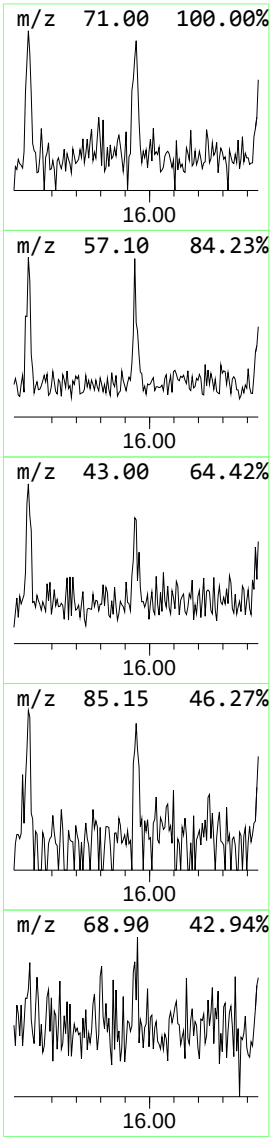
Peak Number 8 unknown15.945 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.945	2.73 ng	33787	Perylene-d12	15.486

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 3-methyl-	226	C16H34	002882-96-4	47
2	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	43
3	Hexadecane	226	C16H34	000544-76-3	43
4	Hexadecane, 7-methyl-	240	C17H36	026730-20-1	38
5	Decane, 5-ethyl-5-methyl-	184	C13H28	017312-74-2	38





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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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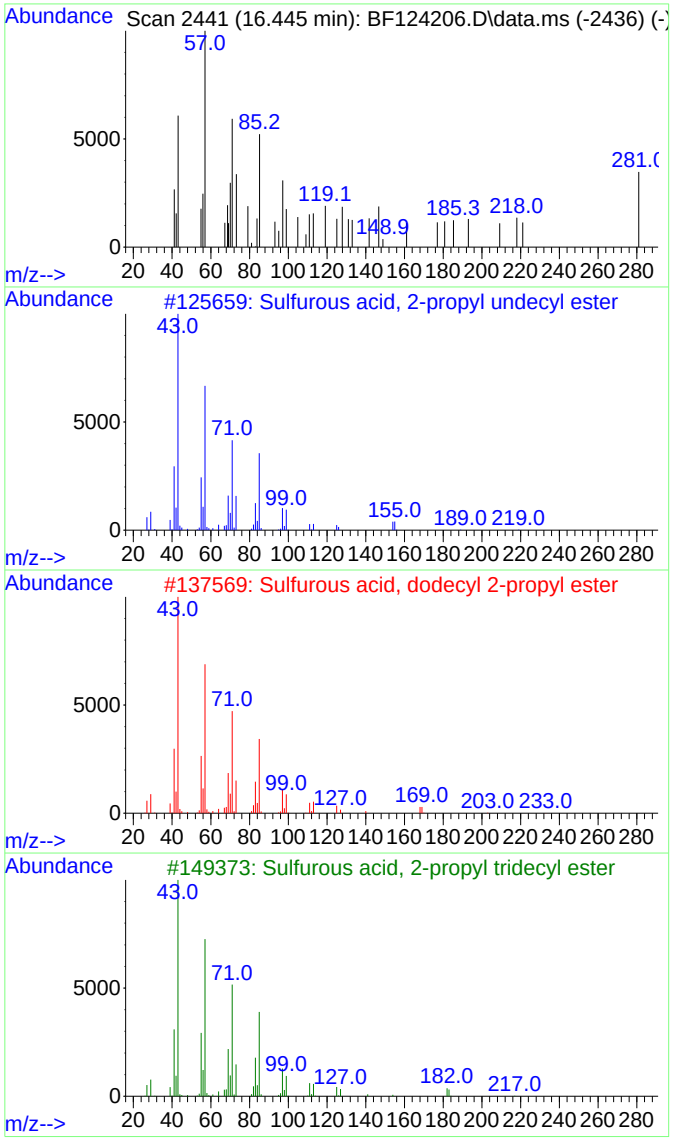
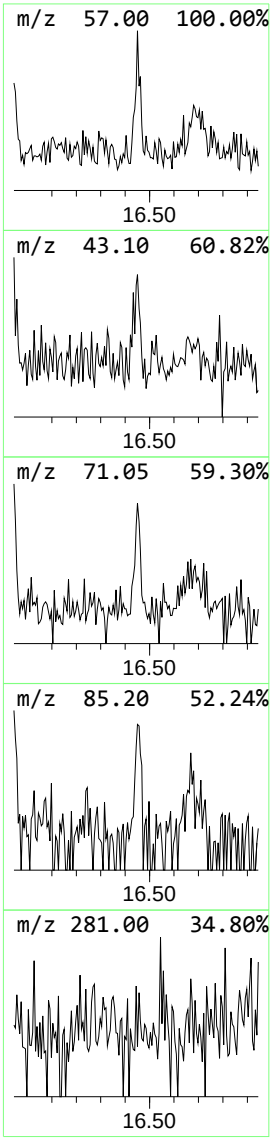
Peak Number 9 unknown16.445 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.445	3.12 ng	38520	Perylene-d12	15.486

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, 2-propyl undecyl...	278	C14H30O3S	1000309-12-2	43
2	Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	43
3	Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	38
4	Decane	142	C10H22	000124-18-5	38
5	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	35





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Acq On : 9 Jun 2021 13:25
Operator : JU/CG
Sample : PB136824BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB136824BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

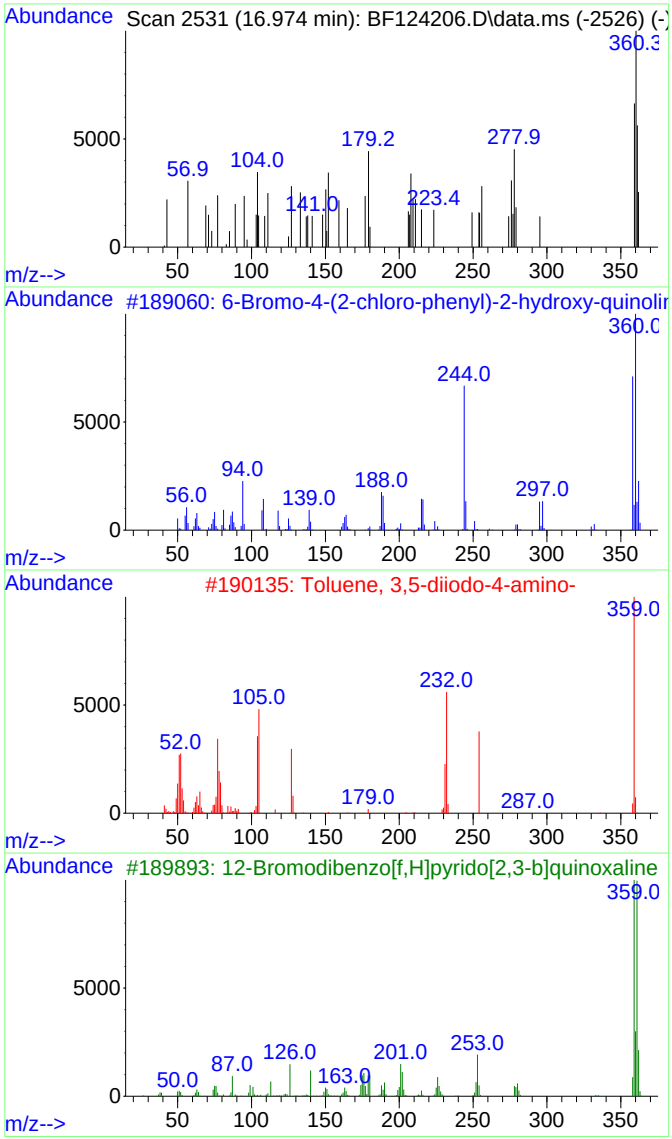
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

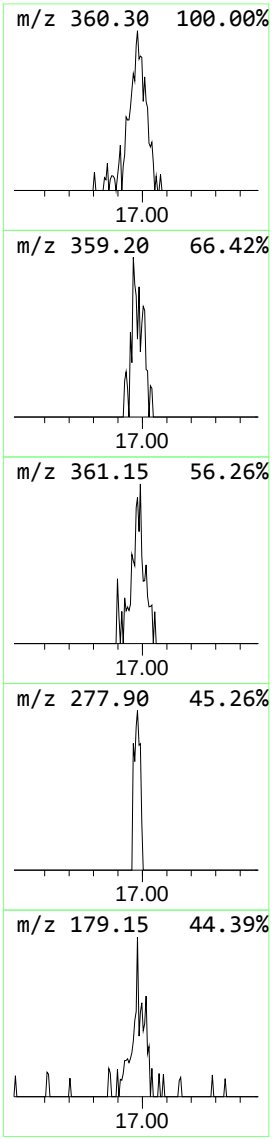
****

Peak Number 10 unknown16.974 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.974	4.28 ng	52852	Perylene-d12	15.486

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Bromo-4-(2-chloro-phenyl)-2-hy...	358	C16H8BrClN2O	284663-85-0	27
2	Toluene, 3,5-diiodo-4-amino-	359	C7H7I2N	064662-57-3	10
3	12-Bromodibenzo[f,H]pyrido[2,3-b...	359	C19H10BrN3	1000332-36-1	10
4	2,6-Diiodo-p-benzoquinone	360	C6H2I2O2	020389-01-9	10
5	Dibenzylidene 4,4'-biphenylenedi...	360	C26H20N2	006311-48-4	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060921\
Data File : BF124206.D
Acq On : 9 Jun 2021 13:25
Operator : JU/CG
Sample : PB136824BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB136824BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
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
Butane, 2-metho...	2.146	5.5	ng	66282	1	6.845	239304	20.0
2-Pentanone, 4-...	5.093	2.1	ng	25299	1	6.845	239304	20.0
Morpholine, 4-p...	13.798	2.1	ng	31076	5	14.010	288689	20.0
unknown13.845	13.845	2.7	ng	38604	5	14.010	288689	20.0
2,2'-(Ethane-1,...	13.874	5.2	ng	75161	5	14.010	288689	20.0
Octadecane	14.780	2.9	ng	35585	6	15.486	247160	20.0
Hentriacontane	15.127	3.1	ng	38985	6	15.486	247160	20.0
unknown15.945	15.945	2.7	ng	33787	6	15.486	247160	20.0
unknown16.445	16.445	3.1	ng	38520	6	15.486	247160	20.0
unknown16.974	16.974	4.3	ng	52852	6	15.486	247160	20.0