LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080724\
Data File : BF138837.D
Acq On : 07 Aug 2024 12:34
Operator : RC/JU
Sample : P3440-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
923-K1-WS-080124

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-BF073024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138837.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	3	7	14	rVB	1646238	2620072	100.00%	21.819%
2	5.057	499	504	513	rVB	35537	51753	1.98%	0.431%
3	5.469	569	574	591	rBV	556120	728710	27.81%	6.068%
4	6.481	740	746	760	rBV	336752	464642	17.73%	3.869%
5	6.840	802	807	812	rVB	234351	290264	11.08%	2.417%
6	7.404	896	903	908	rBV	809900	1093632	41.74%	9.107%
7	8.116	1019	1024	1035	rBV	300236	386151	14.74%	3.216%
8	8.439	1074	1079	1094	rVB	26635	51911	1.98%	0.432%
9	9.192	1201	1207	1212	rBV	1502266	1924826	73.46%	16.029%
10	9.869	1317	1322	1327	rBV	345386	427967	16.33%	3.564%
11	10.251	1382	1387	1391	rBV	52775	74715	2.85%	0.622%
12	10.663	1451	1457	1472	rBV	824962	1085424	41.43%	9.039%
13	11.357	1570	1575	1580	rBV	329527	401665	15.33%	3.345%
14	11.880	1656	1664	1680	rBV2	107918	218285	8.33%	1.818%
15	12.663	1791	1797	1808	rBV	34967	64945	2.48%	0.541%
16	12.939	1838	1844	1849	rBV	1221091	1560424	59.56%	12.994%
17	13.469	1929	1934	1946	rBV2	29425	50328	1.92%	0.419%
18	13.857	1991	2000	2011	rBV3	12306	35042	1.34%	0.292%
19	13.992	2019	2023	2031	rVB	182164	235328	8.98%	1.960%
20	15.457	2266	2272	2281	rVB	156769	242266	9.25%	2.017%

Sum of corrected areas: 12008350

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080724\
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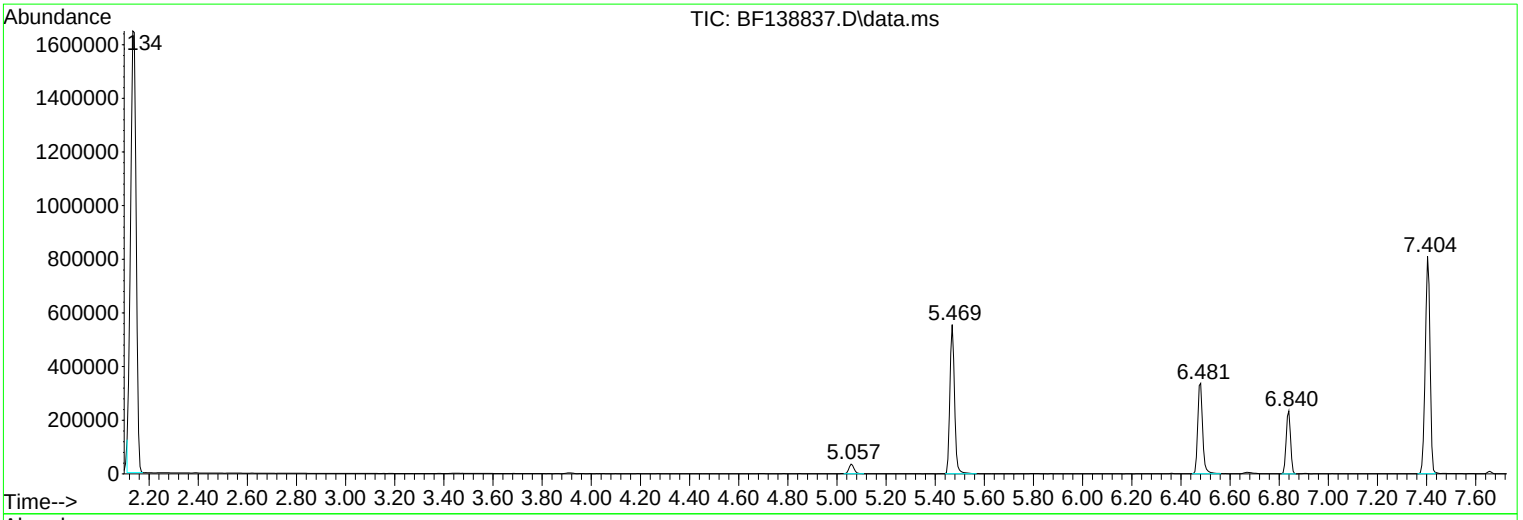
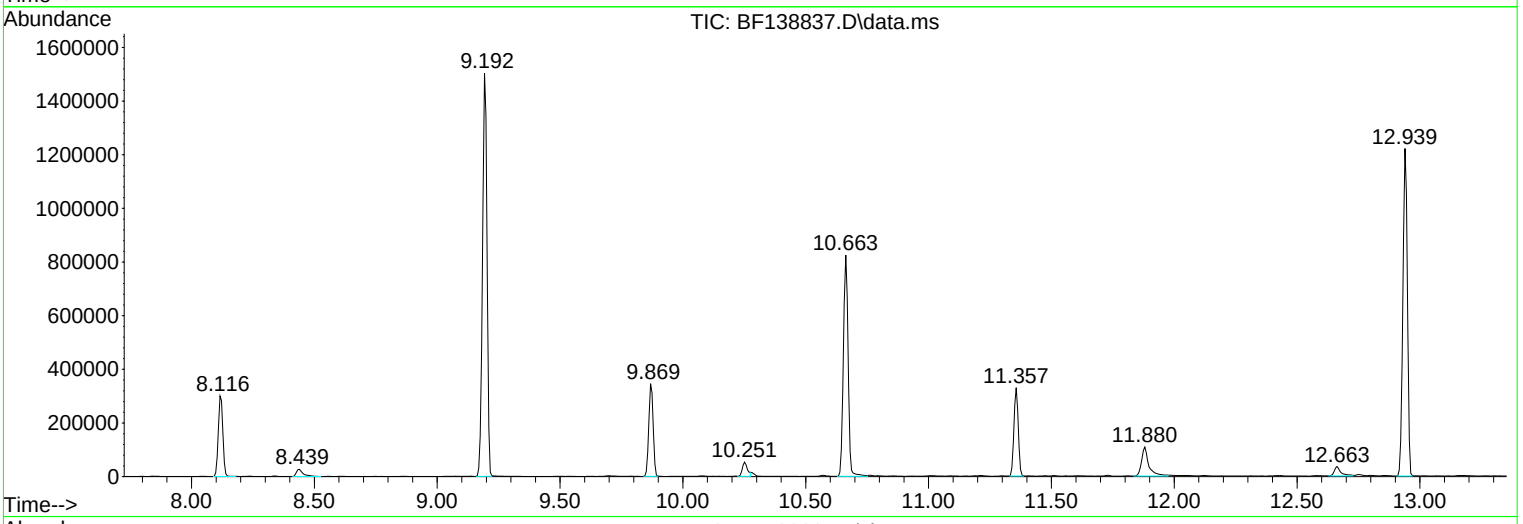
Sample : P3440-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

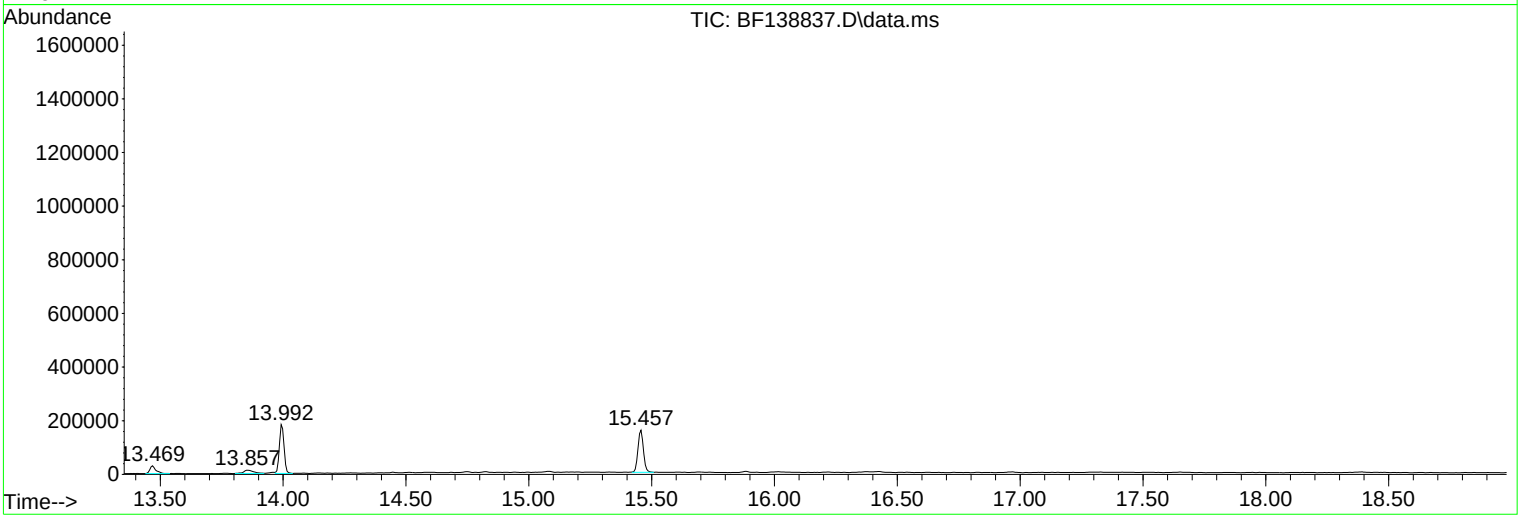
Instrument :
BNA_F
ClientSampleId :
923-K1-WS-080124

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080724\
Data File : BF138837.D
Acq On : 07 Aug 2024 12:34
Operator : RC/JU
Sample : P3440-01
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Instrument :
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923-K1-WS-080124

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

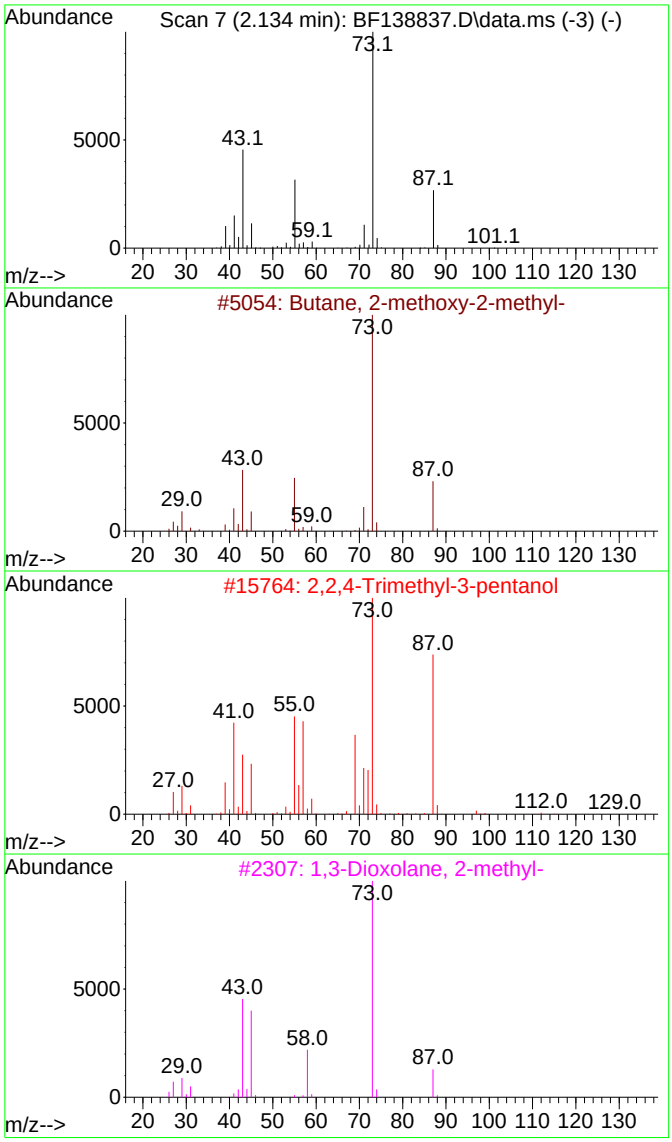
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

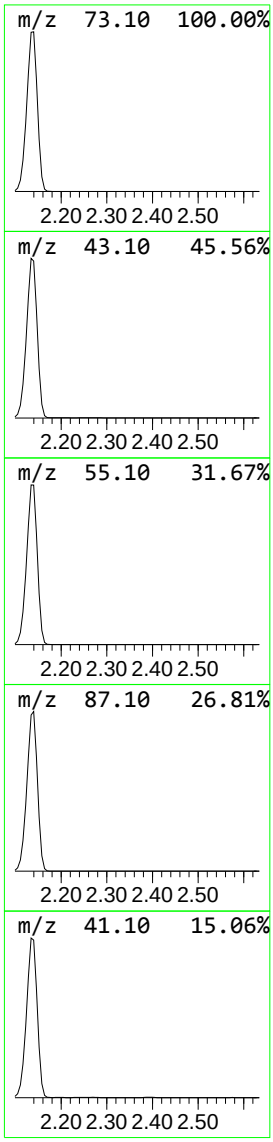
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	180.53 ng	2620070	1,4-Dichlorobenzene-d4	6.840

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080724\
Data File : BF138837.D
Acq On : 07 Aug 2024 12:34
Operator : RC/JU
Sample : P3440-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
923-K1-WS-080124

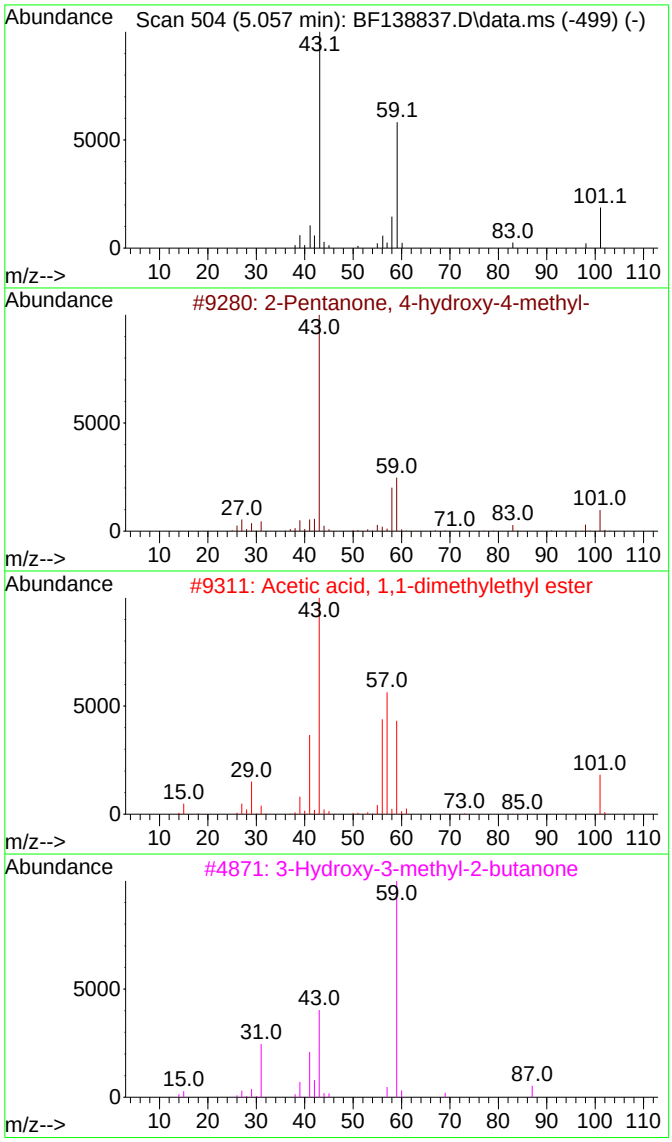
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

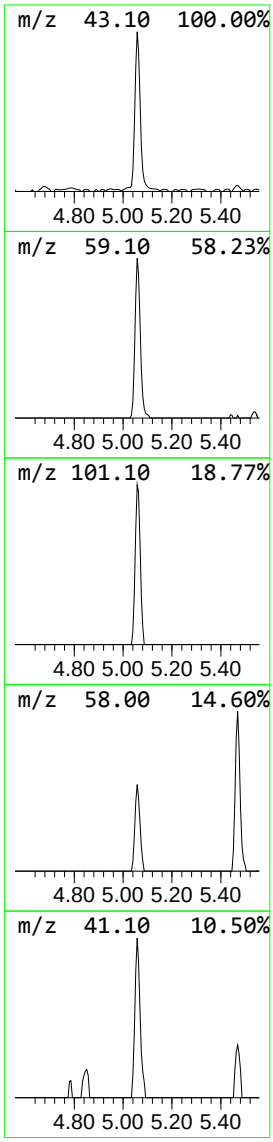
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.057	3.57 ng	51753	1,4-Dichlorobenzene-d4	6.840

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	37
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080724\
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Acq On : 07 Aug 2024 12:34
Operator : RC/JU
Sample : P3440-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
923-K1-WS-080124

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

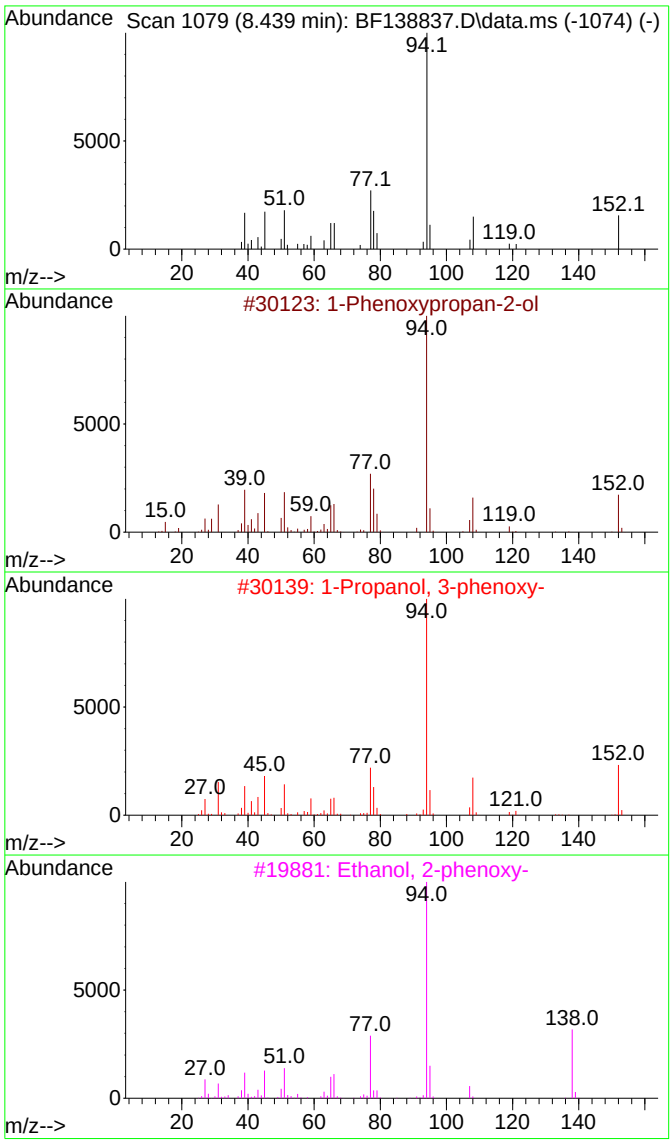
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

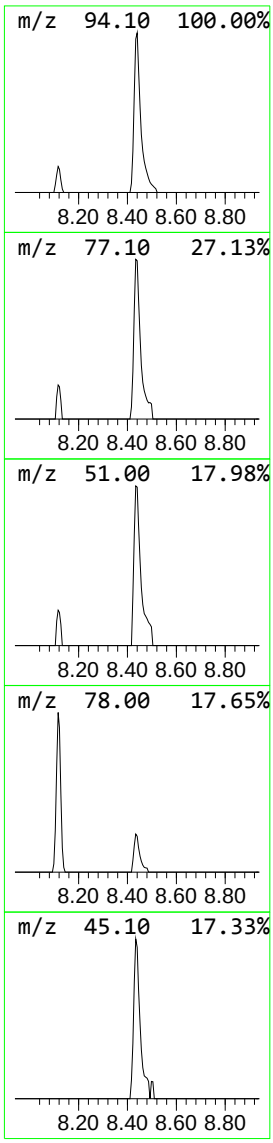
****

Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.439	2.69 ng	51911	Naphthalene-d8	8.116

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	91
3	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4	Benzene, (1,1-dimethylethoxy)-	150	C10H14O	006669-13-2	53
5	2-Hexen-4-yne, 2-methyl-	94	C7H10	058275-93-7	53





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Misc :
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Instrument :
BNA_F
ClientSampleId :
923-K1-WS-080124

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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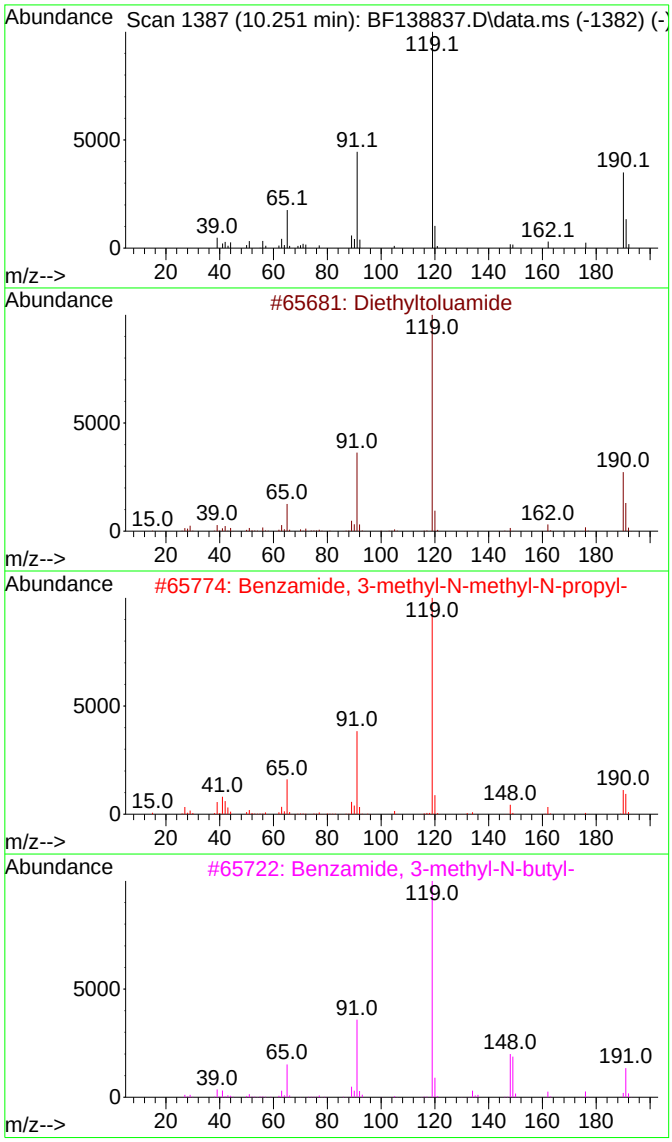
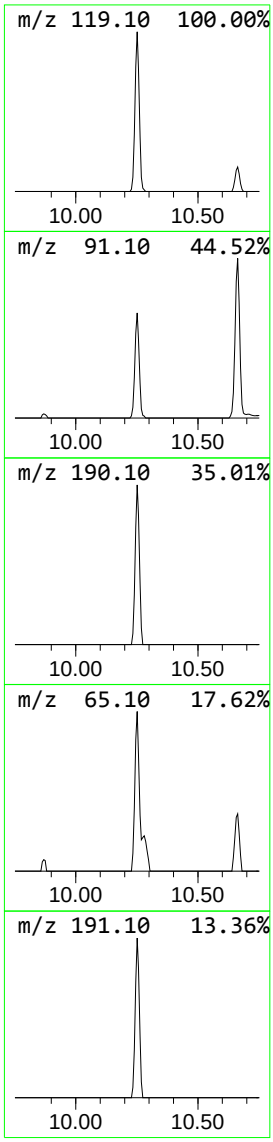
****

Peak Number 4 Diethyltoluamide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.251	3.49 ng	74715	Acenaphthene-d10	9.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyltoluamide	191	C12H17NO	000134-62-3	96
2	Benzamide, 3-methyl-N-methyl-N-p...	191	C12H17NO	1000421-46-2	90
3	Benzamide, 3-methyl-N-butyl-	191	C12H17NO	1000407-41-1	87
4	Benzamide, 2-methyl-N-methyl-N-p...	191	C12H17NO	1000421-44-4	86
5	Benzamide, 4-methyl-N-butyl-	191	C12H17NO	1000407-46-6	83





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Operator : RC/JU
Sample : P3440-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
923-K1-WS-080124

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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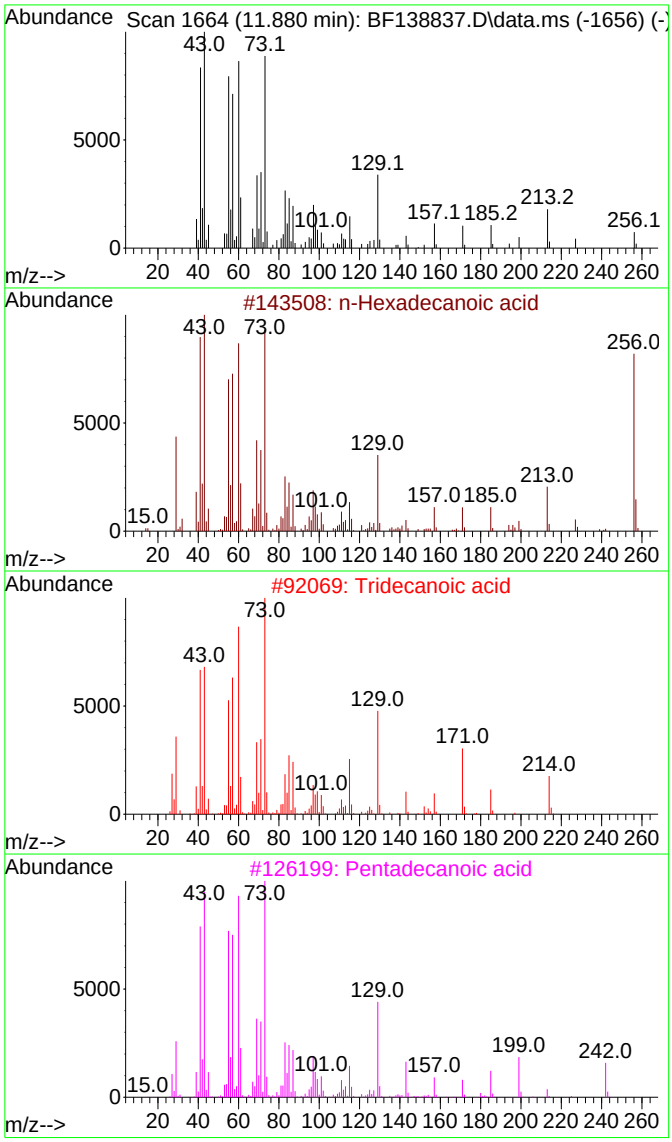
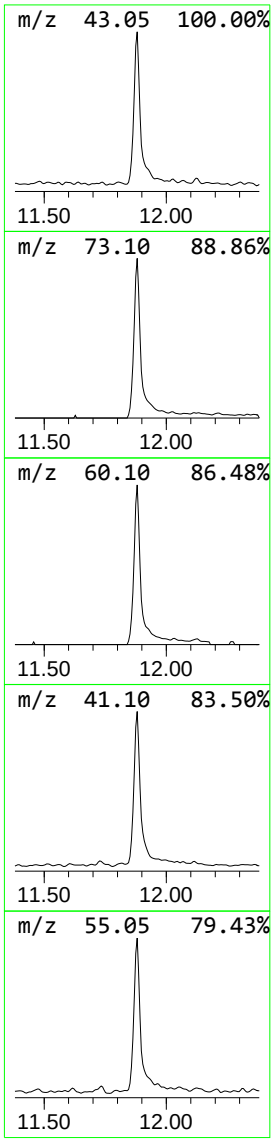
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.880	10.87 ng	218285	Phenanthrene-d10	11.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	96
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	n-Decanoic acid	172	C10H20O2	000334-48-5	83
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080724\
Data File : BF138837.D
Acq On : 07 Aug 2024 12:34
Operator : RC/JU
Sample : P3440-01
Misc :
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Instrument :
BNA_F
ClientSampleId :
923-K1-WS-080124

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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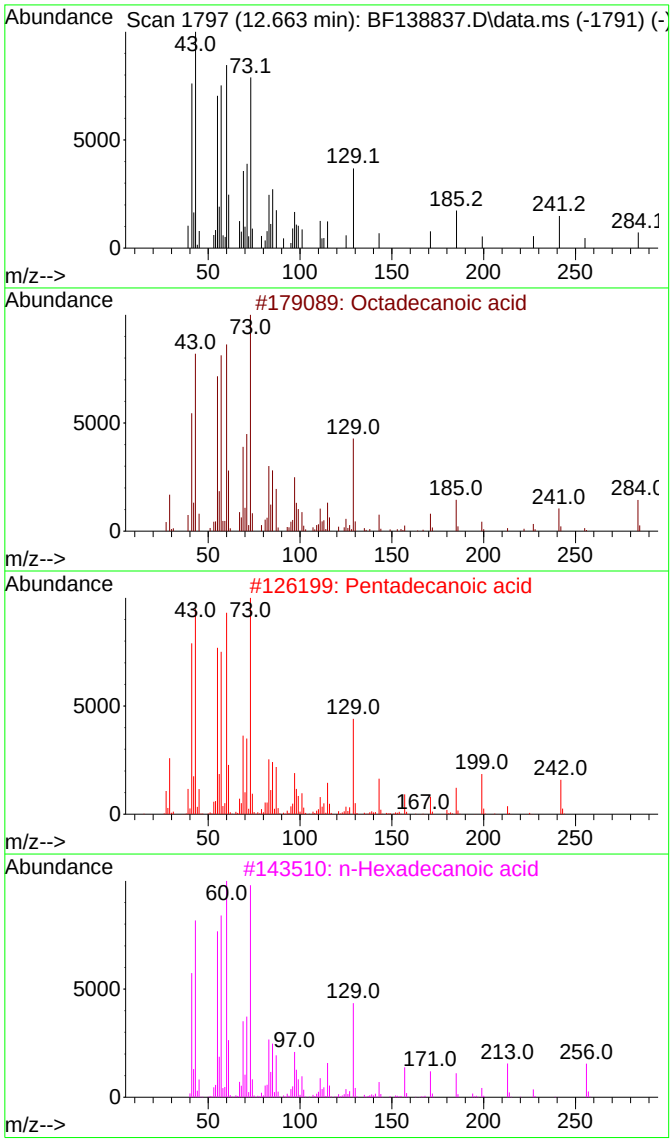
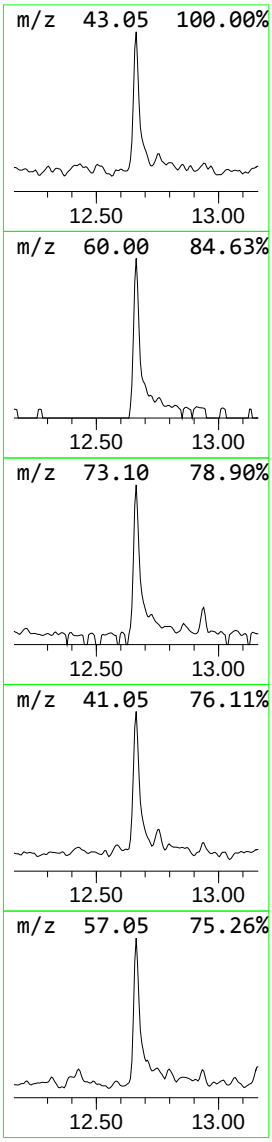
****

Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.663	3.23 ng	64945	Phenanthrene-d10	11.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	91
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	18





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Data File : BF138837.D
Acq On : 07 Aug 2024 12:34
Operator : RC/JU
Sample : P3440-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
923-K1-WS-080124

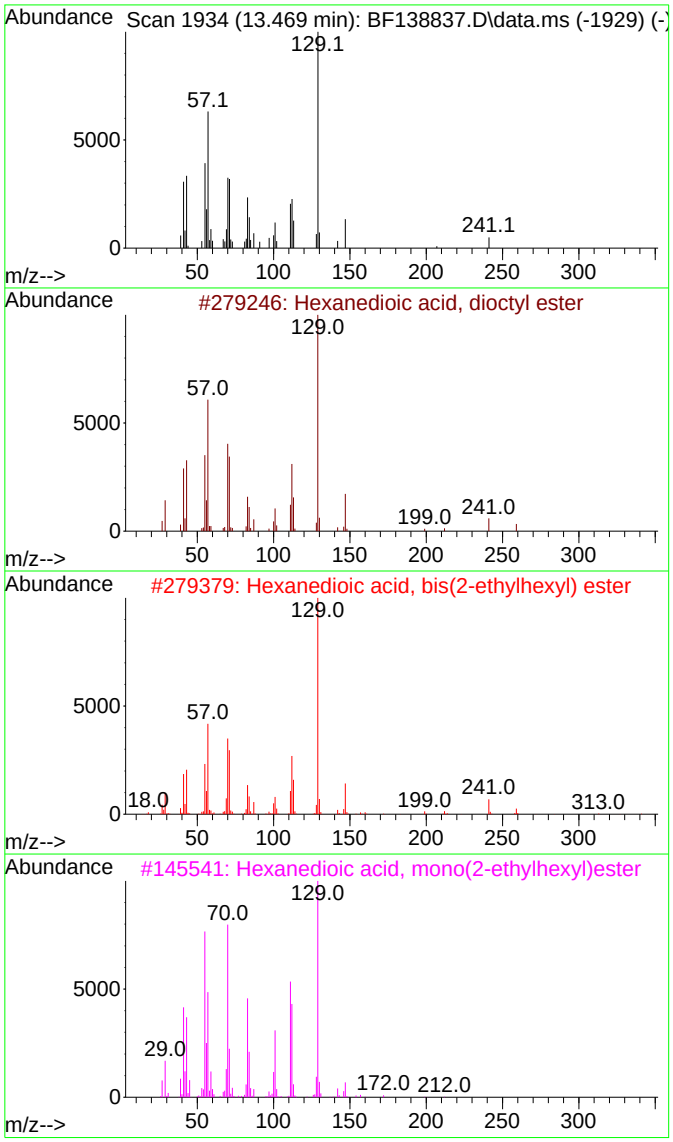
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

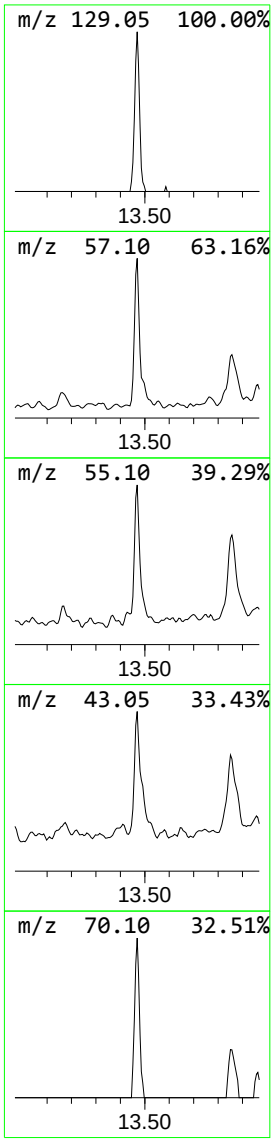
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Hexanedioic acid, dioctyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.469	4.28 ng	50328	Chrysene-d12	13.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	83
2	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	80
3	Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	52
4	Adipic acid, di(oct-4-yl ester)	370	C22H42O4	1000160-80-1	50
5	Adipic acid, cyclopentylmethyl i...	312	C18H32O4	1000324-77-6	47





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Data File : BF138837.D
Acq On : 07 Aug 2024 12:34
Operator : RC/JU
Sample : P3440-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
923-K1-WS-080124

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

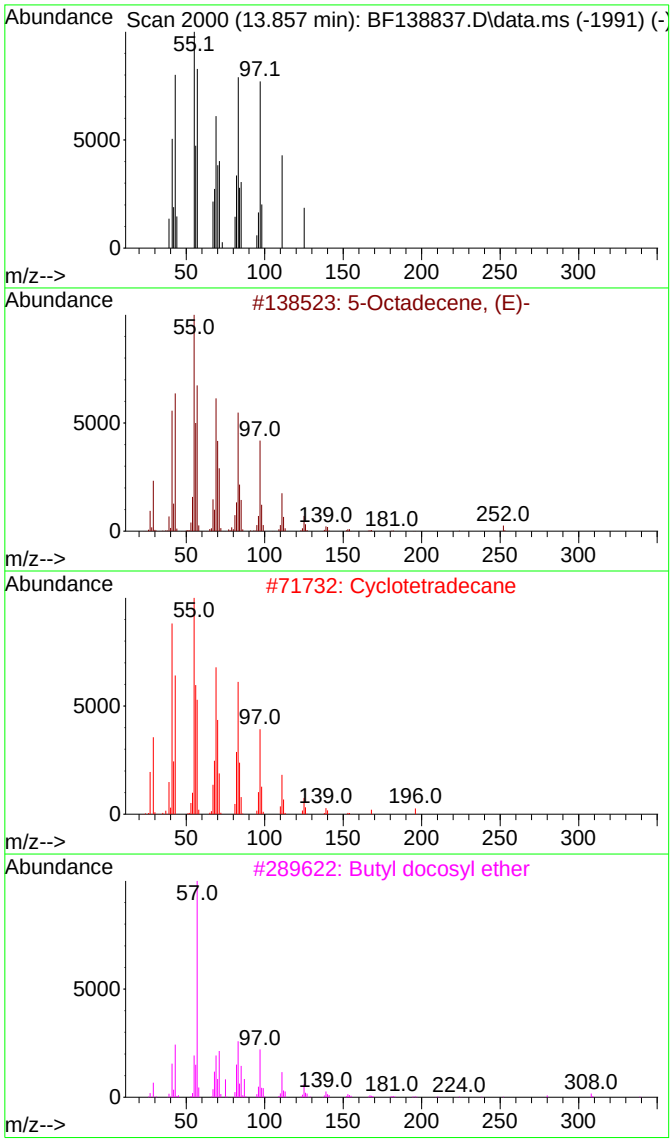
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

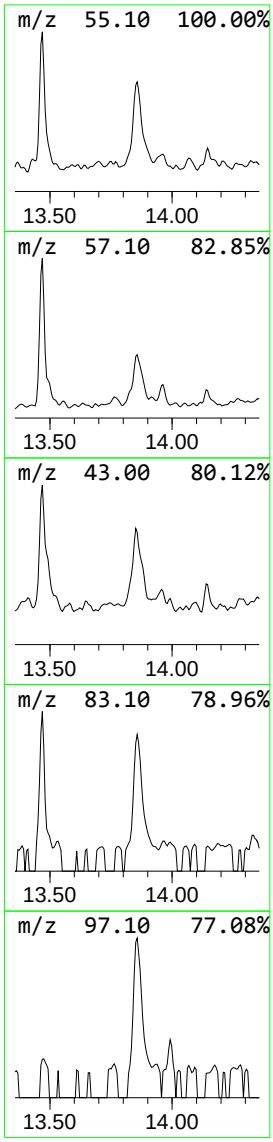
****

Peak Number 8 5-Octadecene, (E)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.857	2.98 ng	35042	Chrysene-d12	13.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	78
2	Cyclotetradecane	196	C14H28	000295-17-0	53
3	Butyl docosyl ether	382	C26H54O	1000406-40-8	50
4	1-Hexacosanol	382	C26H54O	000506-52-5	50
5	Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080724\
Data File : BF138837.D
Acq On : 07 Aug 2024 12:34
Operator : RC/JU
Sample : P3440-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
923-K1-WS-080124

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.134	180.5	ng	2620070	1	6.840	290264	20.0
2-Pentanone, 4-...	5.057	3.6	ng	51753	1	6.840	290264	20.0
1-Phenoxypropan...	8.439	2.7	ng	51911	2	8.116	386151	20.0
Diethyltoluamide	10.251	3.5	ng	74715	3	9.869	427967	20.0
n-Hexadecanoic ...	11.880	10.9	ng	218285	4	11.357	401665	20.0
Octadecanoic acid	12.663	3.2	ng	64945	4	11.357	401665	20.0
Hexanedioic aci...	13.469	4.3	ng	50328	5	13.992	235328	20.0
5-Octadecene, (E)-	13.857	3.0	ng	35042	5	13.992	235328	20.0