LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081024\
Data File : BF138915.D
Acq On : 10 Aug 2024 17:52
Operator : RC/JU
Sample : P3457-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
924-K1-WS-080224

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: BF138915.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	5	11	rVB	1755115	2011955	100.00%	19.692%
2	5.057	499	504	516	rVB	20578	30025	1.49%	0.294%
3	5.469	569	574	595	rBV	420868	579414	28.80%	5.671%
4	6.481	742	746	770	rVB	257973	364518	18.12%	3.568%
5	6.840	802	807	812	rBV	203504	253743	12.61%	2.484%
6	7.404	897	903	908	rBV	730370	966670	48.05%	9.461%
7	8.116	1019	1024	1038	rBV	260653	336817	16.74%	3.297%
8	8.434	1074	1078	1090	rVB	36294	52586	2.61%	0.515%
9	9.192	1201	1207	1212	rBV	1403496	1762695	87.61%	17.252%
10	9.869	1317	1322	1333	rVB	308524	389401	19.35%	3.811%
11	10.251	1383	1387	1392	rBV	36564	45612	2.27%	0.446%
12	10.663	1452	1457	1471	rBV	759388	990553	49.23%	9.695%
13	11.357	1570	1575	1588	rBV	309819	383896	19.08%	3.757%
14	11.880	1659	1664	1679	rBV2	28130	52179	2.59%	0.511%
15	12.598	1779	1786	1793	rBV2	14893	22984	1.14%	0.225%
16	12.751	1808	1812	1817	rVB	48109	57284	2.85%	0.561%
17	12.939	1839	1844	1849	rBV	1038932	1293374	64.28%	12.659%
18	13.457	1926	1932	1936	rBV	26825	35354	1.76%	0.346%
19	13.827	1990	1995	2008	rBV	33378	65326	3.25%	0.639%
20	13.998	2019	2024	2031	rVB	153488	192683	9.58%	1.886%
21	14.821	2160	2164	2168	rBV	15043	26933	1.34%	0.264%
22	14.974	2181	2190	2198	rBV5	24361	76102	3.78%	0.745%
23	15.463	2267	2273	2288	rVB	142676	226992	11.28%	2.222%

Sum of corrected areas: 10217096

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081024\
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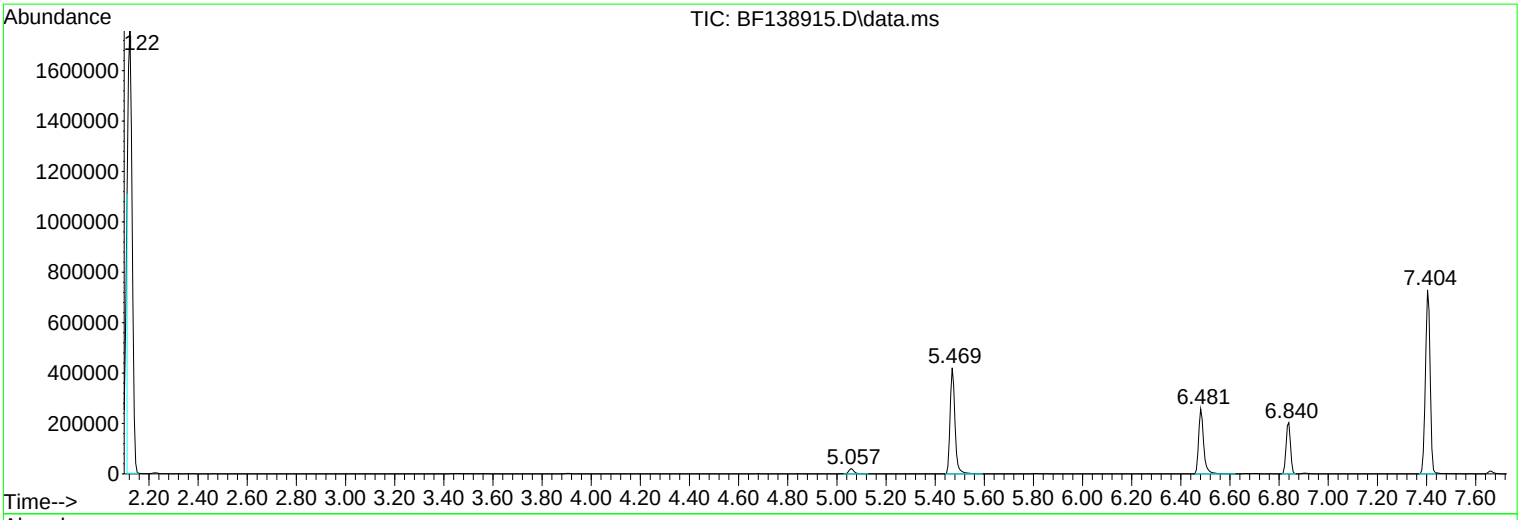
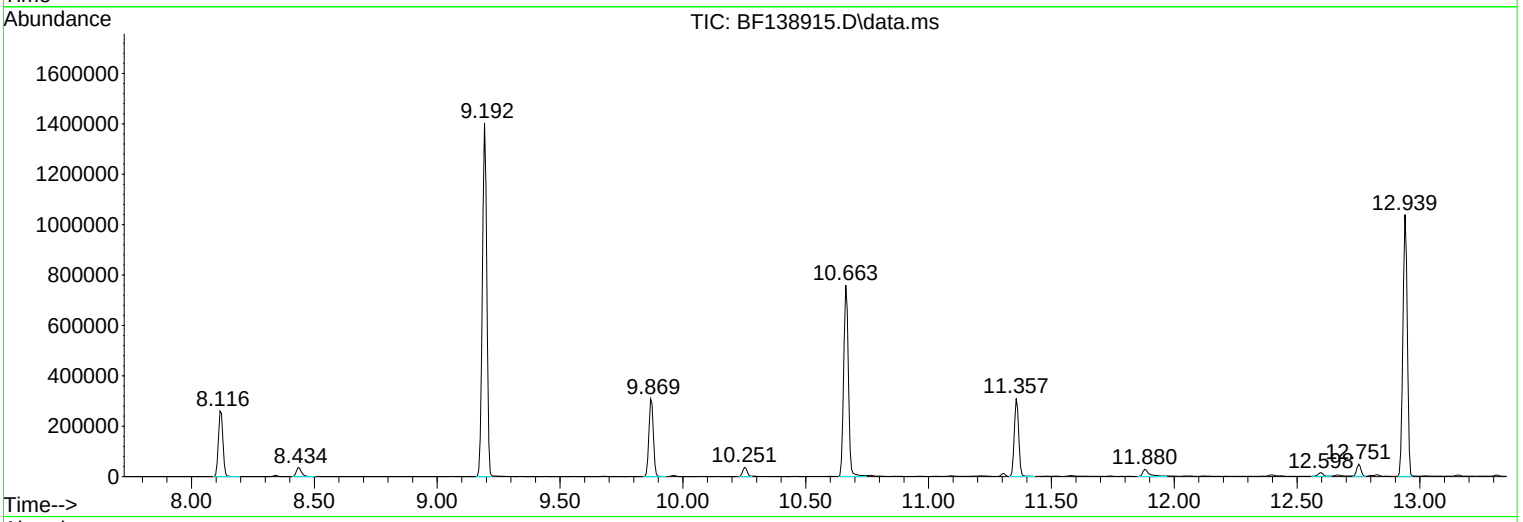
Misc :
ALS Vial : 16 Sample Multiplier: 1

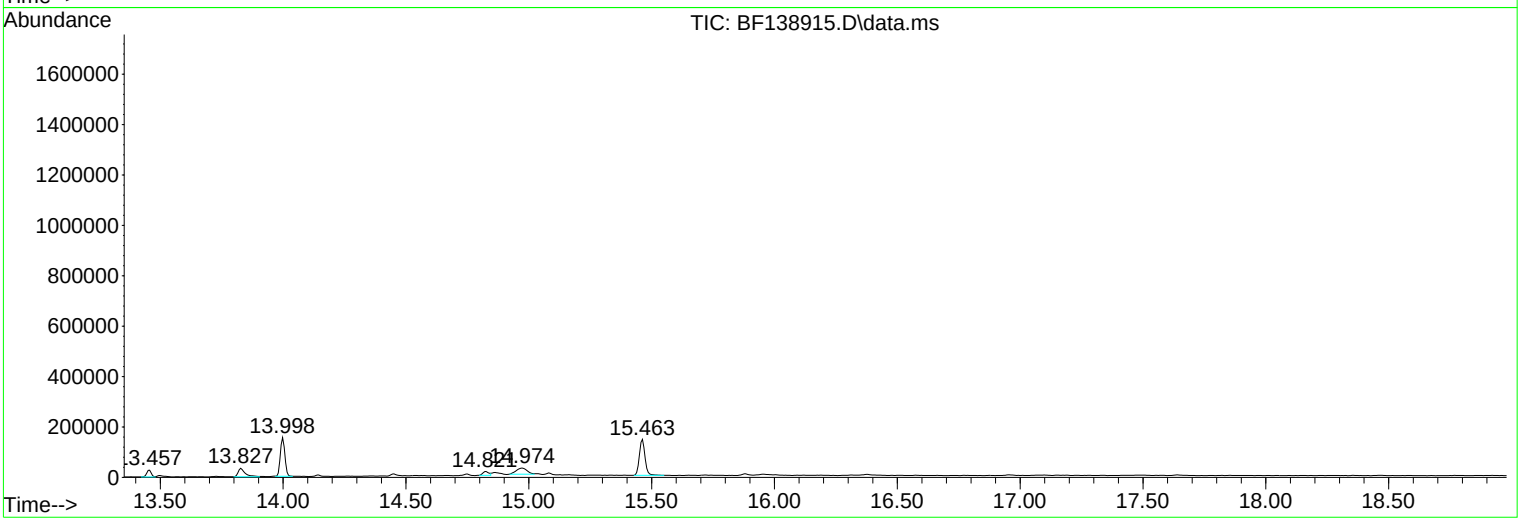
Instrument :
BNA_F
ClientSampleId :
924-K1-WS-080224

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







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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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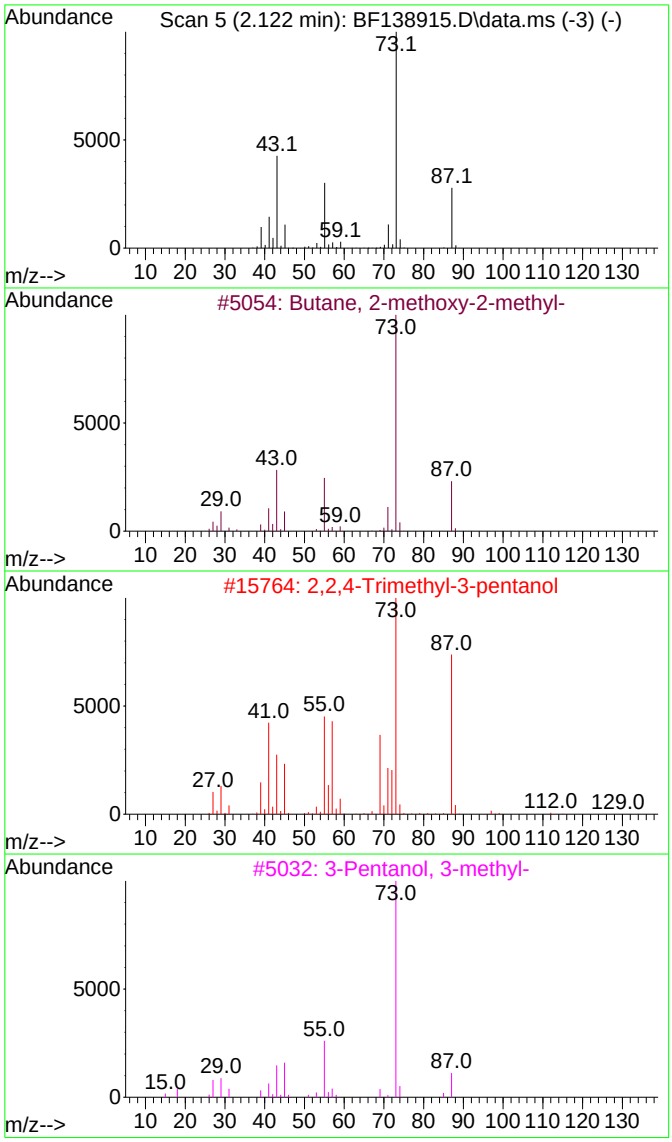
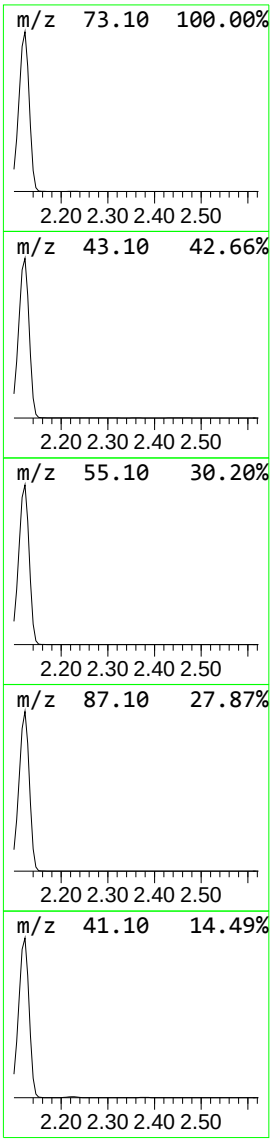
****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.122	158.58 ng	2011960	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	39
3	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	17
4	Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	17
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12





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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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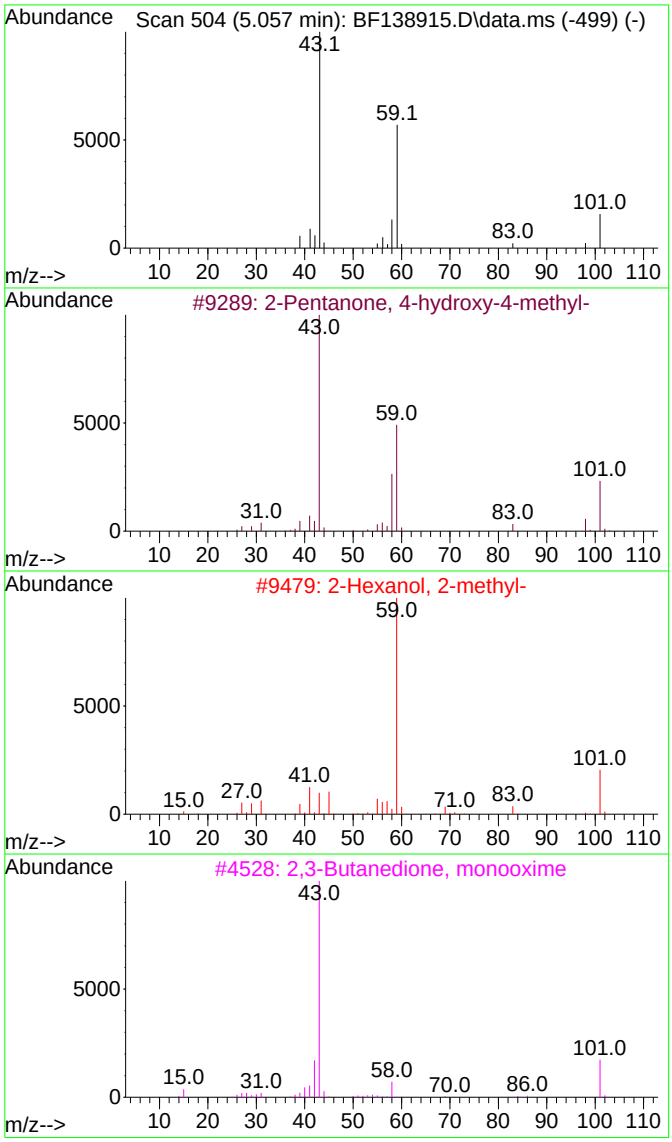
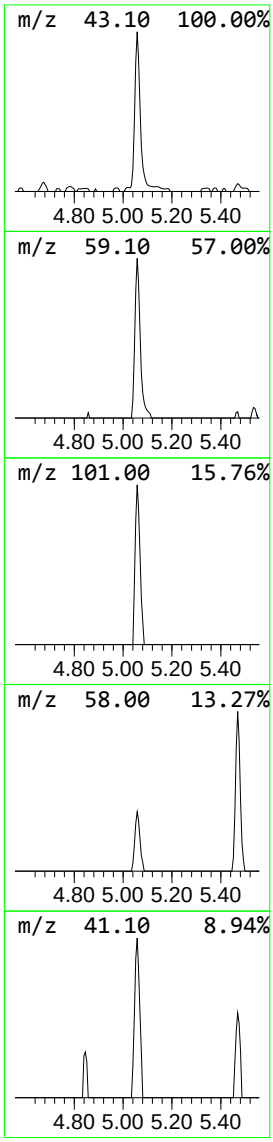
****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.057	2.37 ng	30025	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	72
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9





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Operator : RC/JU
Sample : P3457-01
Misc :
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Instrument :
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ClientSampleId :
924-K1-WS-080224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
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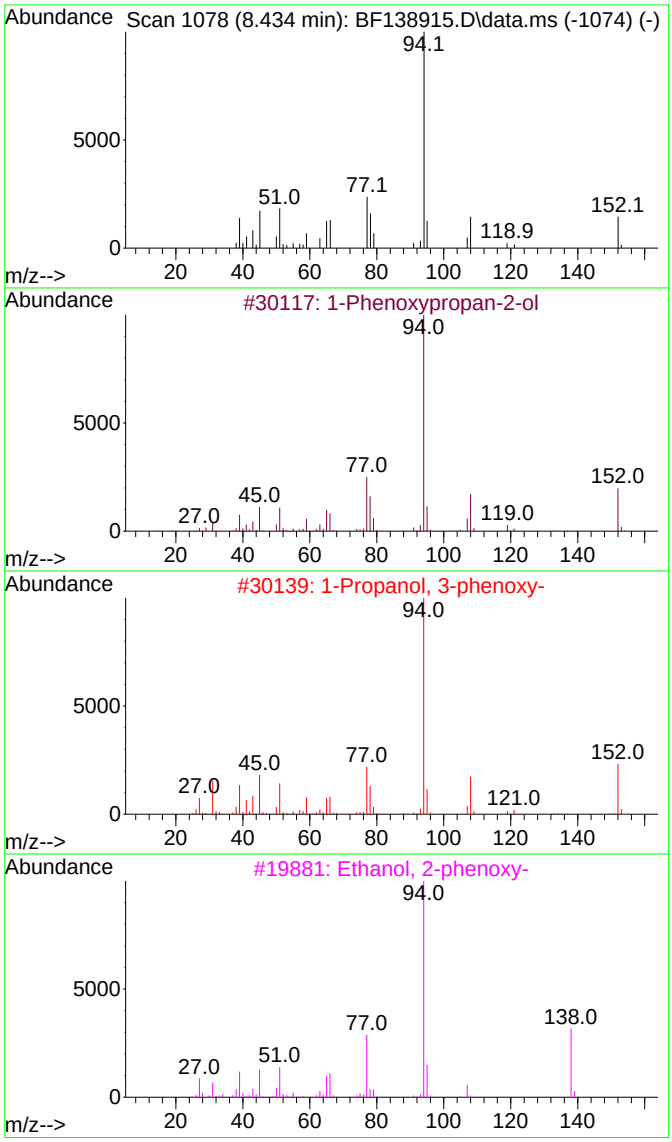
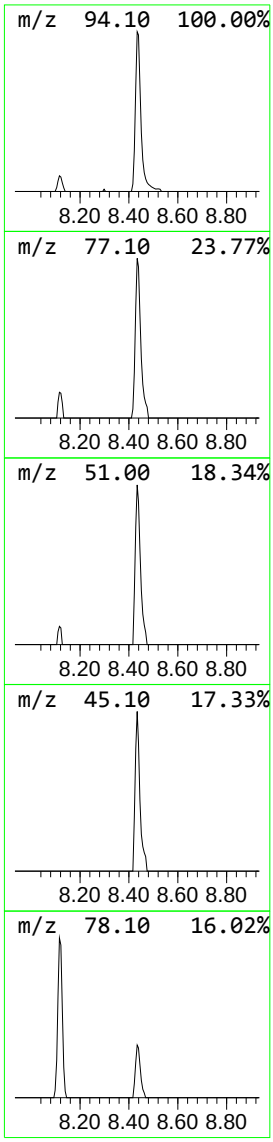
****

Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.434	3.12 ng	52586	Naphthalene-d8	8.116

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	97
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	91
3	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
5	Benzene, (1,1-dimethylethoxy)-	150	C10H14O	006669-13-2	53





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Instrument :
BNA_F
ClientSampleId :
924-K1-WS-080224

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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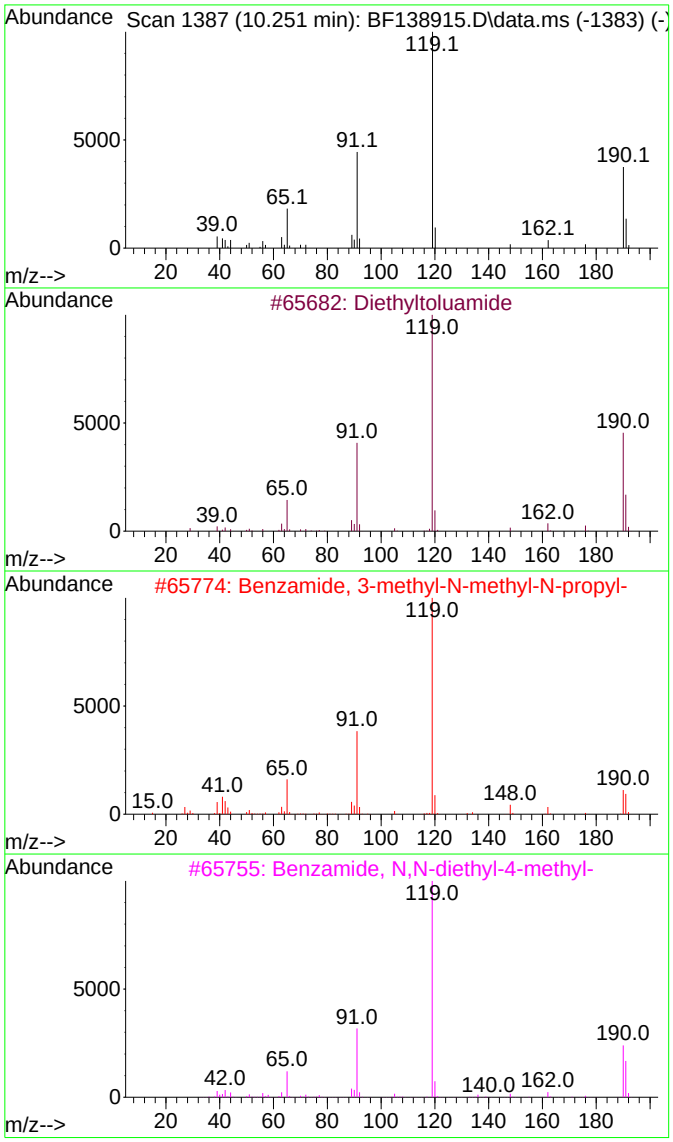
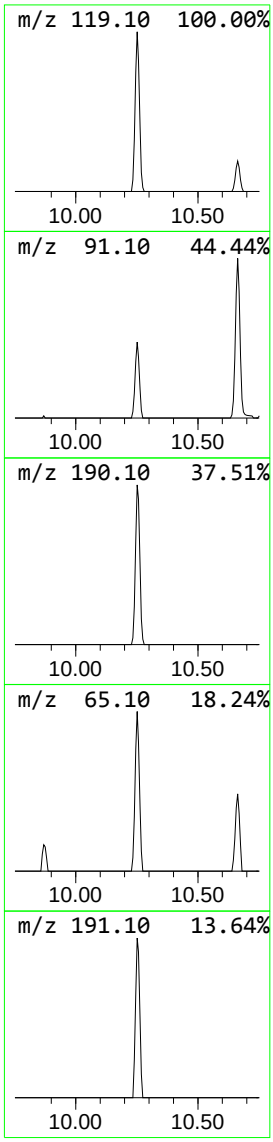
****

Peak Number 4 Diethyltoluamide Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.251	2.34 ng	45612	Acenaphthene-d10	9.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyltoluamide	191	C12H17NO	000134-62-3	94
2	Benzamide, 3-methyl-N-methyl-N-p...	191	C12H17NO	1000421-46-2	90
3	Benzamide, N,N-diethyl-4-methyl-	191	C12H17NO	002728-05-4	83
4	Benzamide, 2-methyl-N-methyl-N-p...	191	C12H17NO	1000421-44-4	83
5	Benzamide, 3-methyl-N-butyl-	191	C12H17NO	1000407-41-1	80





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Sample : P3457-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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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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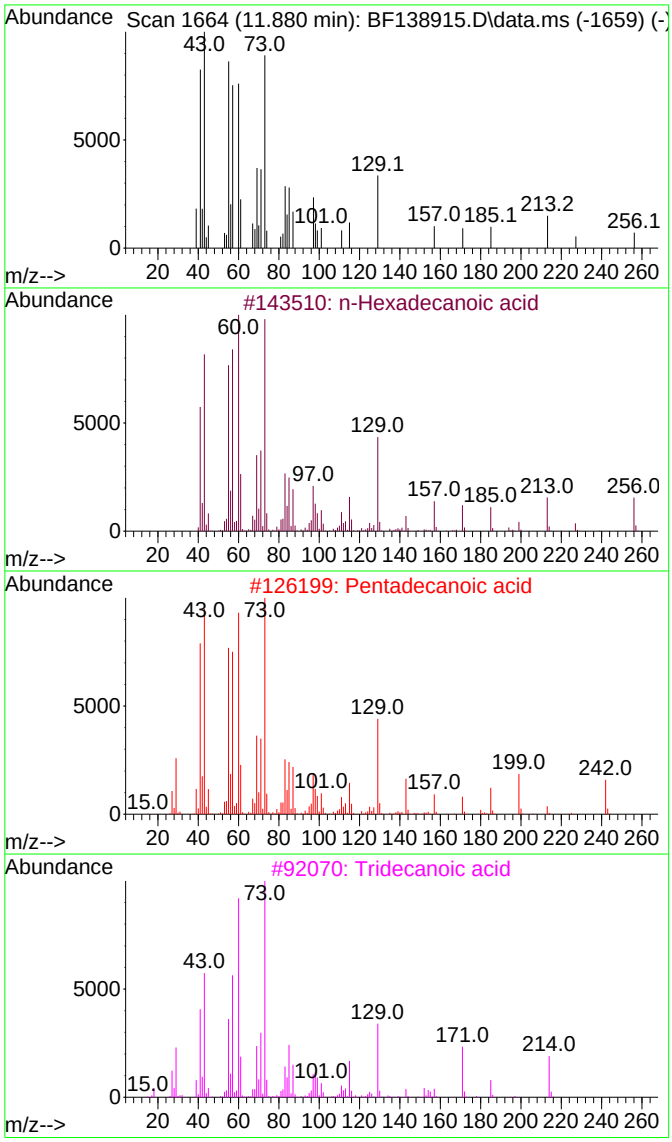
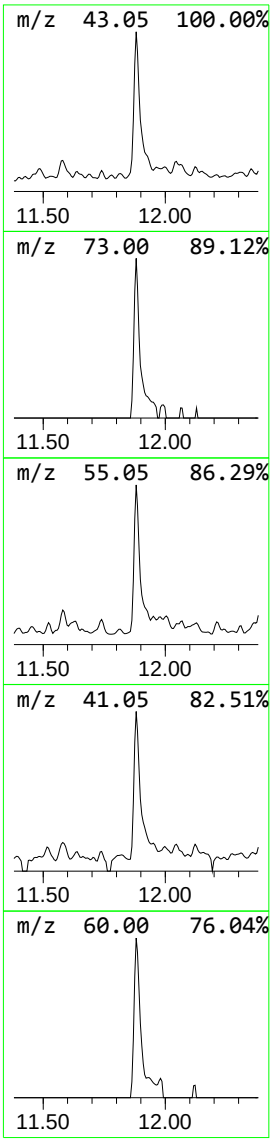
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.881	2.72 ng	52179	Phenanthrene-d10	11.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Tridecanoic acid	214	C13H26O2	000638-53-9	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	59





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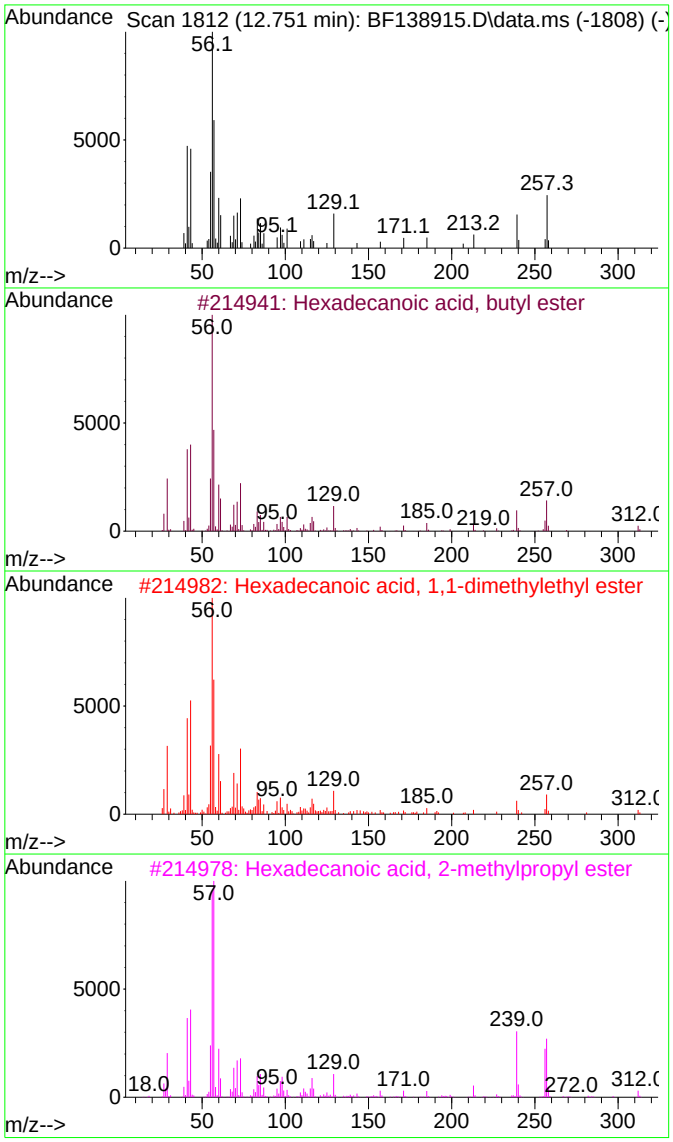
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

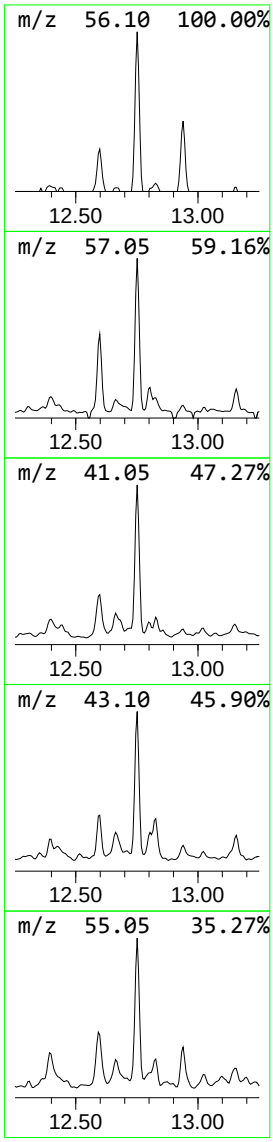
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.751	5.95 ng	57284	Chrysene-d12	13.998

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	90
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	64
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	43
4	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	27
5	1-Hexene, 3,4-dimethyl-	112	C8H16	016745-94-1	27





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Sample : P3457-01
Misc :
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Instrument :
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ClientSampleId :
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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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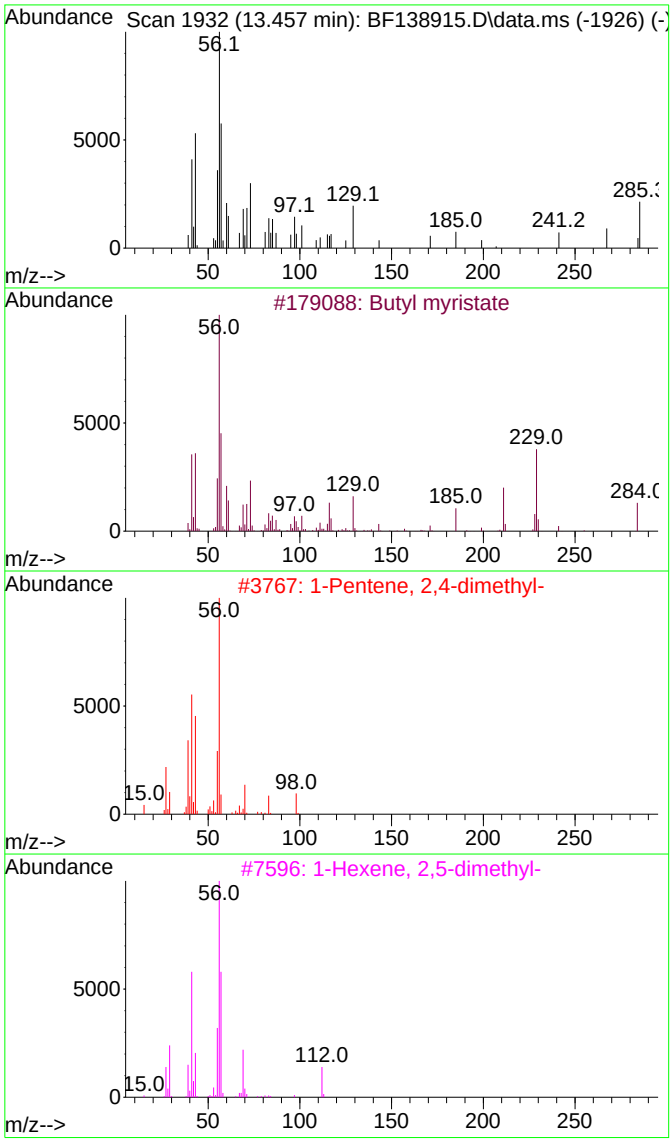
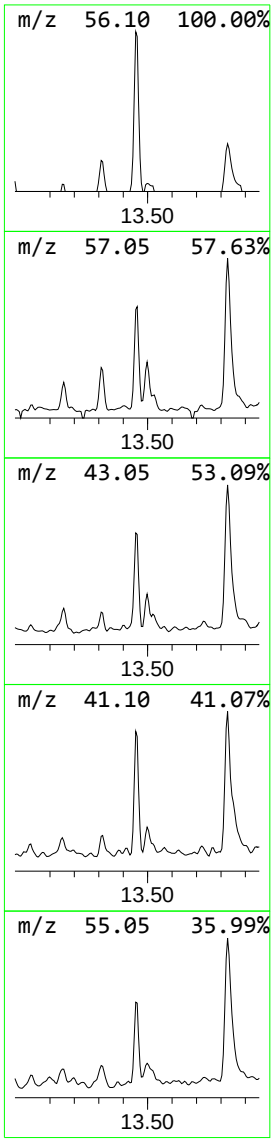
Peak Number 7 Butyl myristate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.457	3.67 ng	35354	Chrysene-d12	13.998

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl myristate	284	C18H36O2	000110-36-1	72
2	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	27
3	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27
4	1-Hexene, 5-methyl-	98	C7H14	003524-73-0	27
5	Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	25





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TIC Library : C:\Database\NIST20.L
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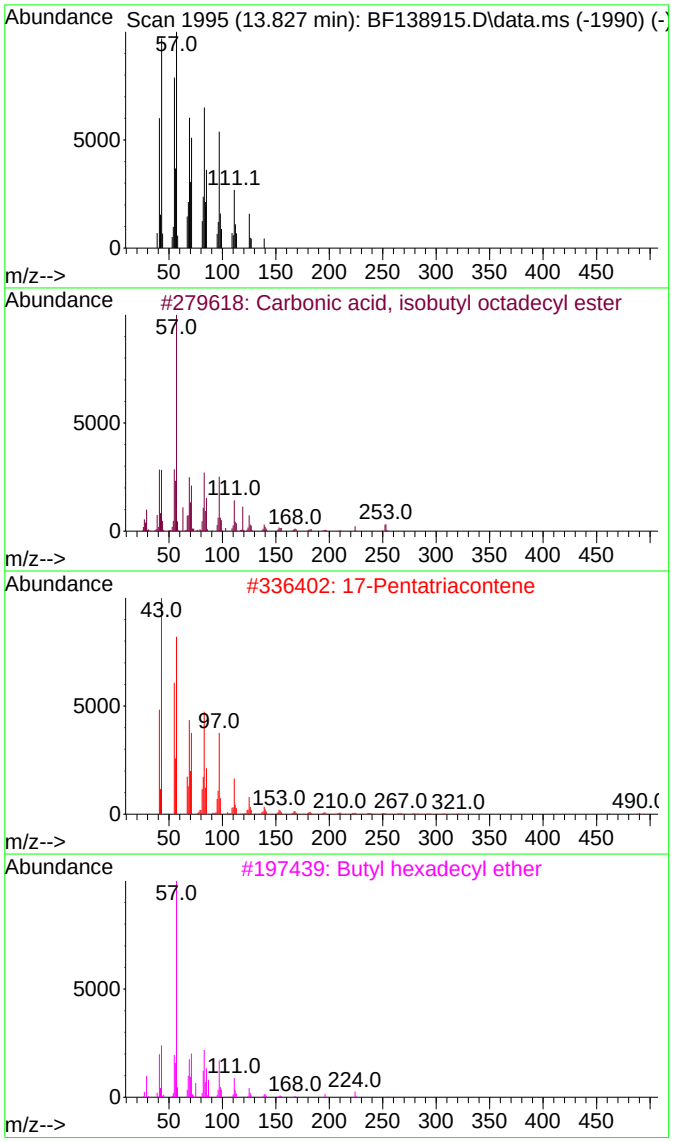
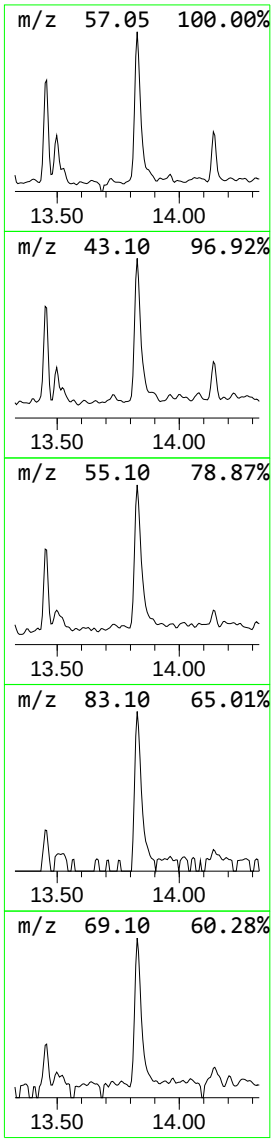
Peak Number 8 Carbonic acid, isobutyl oct... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.827	6.78 ng	65326	Chrysene-d12	13.998

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	91
2	17-Pentatriacontene	491	C35H70	006971-40-0	90
3	Butyl hexadecyl ether	298	C20H42O	1010406-40-5	90
4	Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	90
5	1-Docosene	308	C22H44	001599-67-3	87





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Acq On : 10 Aug 2024 17:52
Operator : RC/JU
Sample : P3457-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
924-K1-WS-080224

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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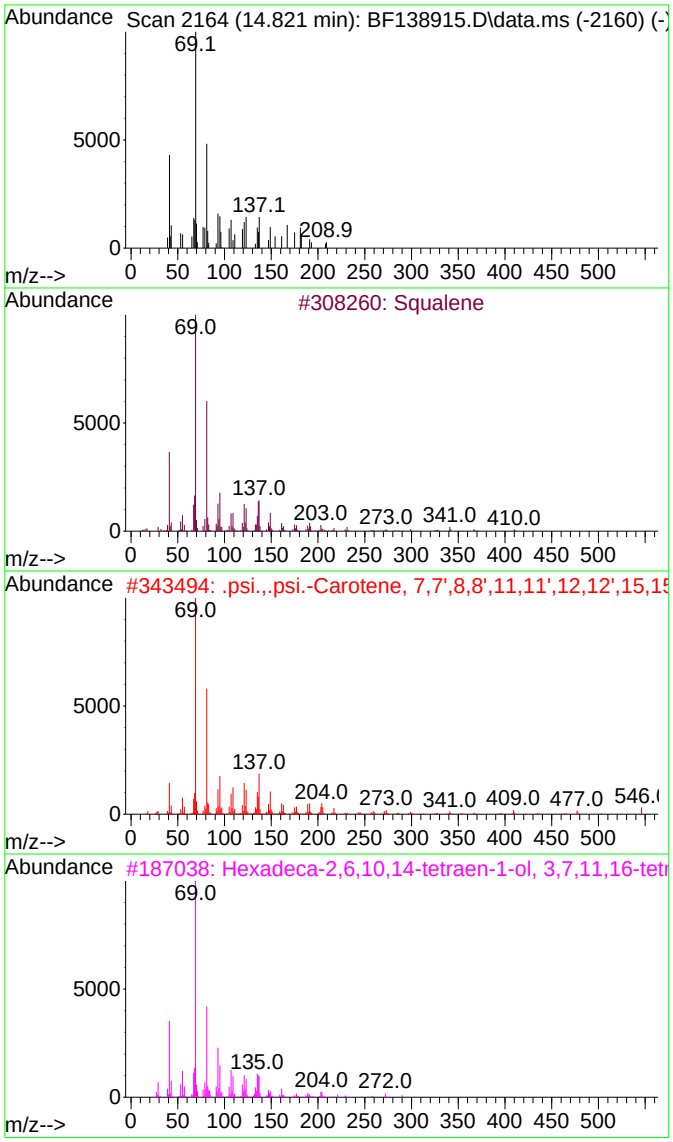
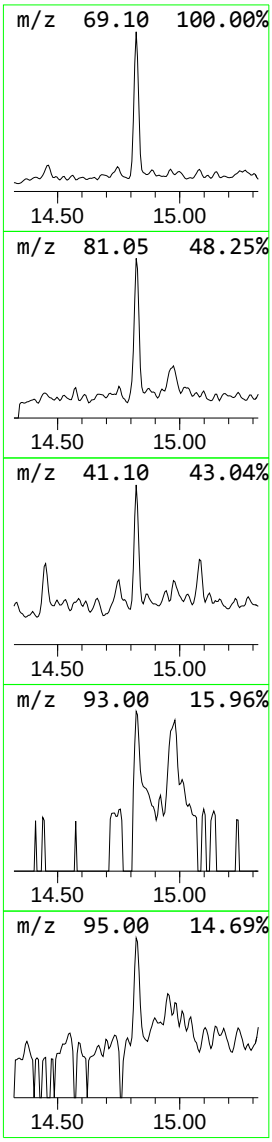
Peak Number 9 Squalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.822	2.37 ng	26933	Perylene-d12	15.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	80
2	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	80
3	Hexadeca-2,6,10,14-tetraen-1-ol,...	290	C20H34O	007614-21-3	72
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	59
5	Supraene	410	C30H50	007683-64-9	53





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Data File : BF138915.D
Acq On : 10 Aug 2024 17:52
Operator : RC/JU
Sample : P3457-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
924-K1-WS-080224

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

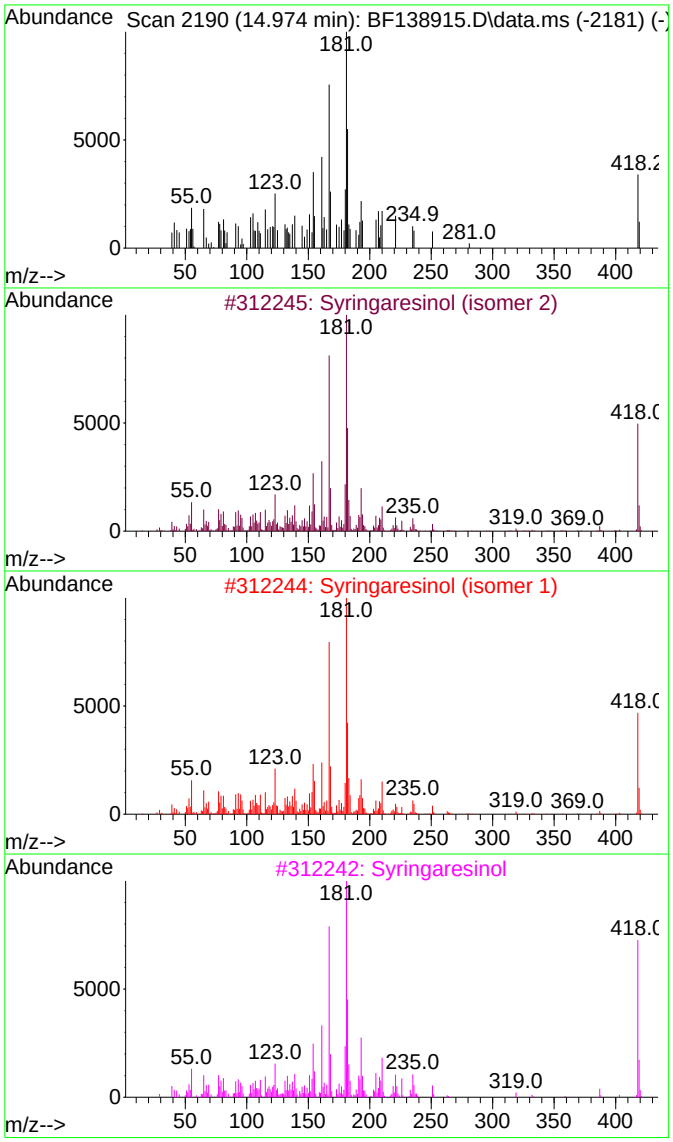
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

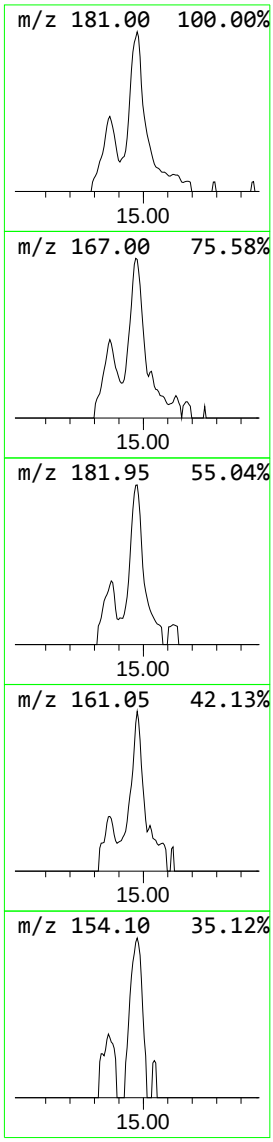
****

Peak Number 10 Syringaresinol (isomer 2) Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.974	6.71 ng	76102	Perylene-d12	15.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Syringaresinol (isomer 2)	418	C22H26O8	1000495-97-1	96
2	Syringaresinol (isomer 1)	418	C22H26O8	1000495-97-0	94
3	Syringaresinol	418	C22H26O8	000487-35-4	91
4	1,4-benzenediamine, N4,N4-diethy...	182	C10H15FN2	1000404-88-0	30
5	Benzene, 1-methyl-3-(phenylmethyl)-	182	C14H14	000620-47-3	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081024\
Data File : BF138915.D
Acq On : 10 Aug 2024 17:52
Operator : RC/JU
Sample : P3457-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
924-K1-WS-080224

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...	2.122	158.6	ng	2011960	1	6.840	253743	20.0
2-Pentanone, 4-...	5.057	2.4	ng	30025	1	6.840	253743	20.0
1-Phenoxypropan...	8.434	3.1	ng	52586	2	8.116	336817	20.0
Diethyltoluamide	10.251	2.3	ng	45612	3	9.869	389401	20.0
n-Hexadecanoic ...	11.881	2.7	ng	52179	4	11.357	383896	20.0
Hexadecanoic ac...	12.751	6.0	ng	57284	5	13.998	192683	20.0
Butyl myristate	13.457	3.7	ng	35354	5	13.998	192683	20.0
Carbonic acid, ...	13.827	6.8	ng	65326	5	13.998	192683	20.0
Squalene	14.822	2.4	ng	26933	6	15.463	226992	20.0
Syringaresinol ...	14.974	6.7	ng	76102	6	15.463	226992	20.0