LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080924\
Data File : BF138891.D
Acq On : 09 Aug 2024 16:33
Operator : RC/JU
Sample : P3469-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MLS-15-625-640

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: BF138891.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	1705961	1935100	86.30%	14.885%
2	2.922	134	141	153	rBB	34698	62706	2.80%	0.482%
3	3.899	301	307	318	rBB	99651	160402	7.15%	1.234%
4	5.057	499	504	518	rVB	27362	41446	1.85%	0.319%
5	5.469	569	574	592	rVB	465370	631052	28.14%	4.854%
6	5.787	623	628	637	rBV	179762	240069	10.71%	1.847%
7	6.481	741	746	762	rBV	283311	395526	17.64%	3.042%
8	6.840	802	807	813	rVB	218130	271617	12.11%	2.089%
9	7.404	895	903	908	rBV	785631	1062478	47.38%	8.173%
10	8.116	1019	1024	1038	rVB	284175	364728	16.27%	2.806%
11	8.340	1057	1062	1063	rBV	37536	50762	2.26%	0.390%
12	8.357	1063	1065	1074	rVV	54437	88359	3.94%	0.680%
13	8.434	1074	1078	1089	rVB	25802	42699	1.90%	0.328%
14	9.192	1201	1207	1212	rBV	1562527	2036344	90.81%	15.664%
15	9.869	1317	1322	1332	rVB	351740	433747	19.34%	3.336%
16	9.963	1332	1338	1360	rBV	335866	521651	23.26%	4.013%
17	10.604	1440	1447	1452	rVB	18459	22672	1.01%	0.174%
18	10.663	1452	1457	1471	rBV	753537	998721	44.54%	7.682%
19	11.304	1562	1566	1569	rBV	23583	25630	1.14%	0.197%
20	11.357	1570	1575	1585	rVV	395038	492313	21.96%	3.787%
21	12.445	1747	1760	1766	rBV	71877	136685	6.10%	1.051%
22	12.569	1777	1781	1786	rBV3	19667	33308	1.49%	0.256%
23	12.686	1797	1801	1808	rVB	30431	42160	1.88%	0.324%
24	12.804	1814	1821	1827	rBV5	12254	26579	1.19%	0.204%
25	12.945	1838	1845	1850	rVB	1664157	2242360	100.00%	17.249%
26	13.998	2020	2024	2031	rVV	225975	285963	12.75%	2.200%
27	14.075	2033	2037	2041	rVB	27934	34257	1.53%	0.264%
28	14.822	2159	2164	2169	rBV	55865	73991	3.30%	0.569%
29	15.463	2267	2273	2289	rVB	132832	219775	9.80%	1.691%
30	15.639	2297	2303	2310	rVB	17085	27132	1.21%	0.209%

Sum of corrected areas: 13000232

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080924\
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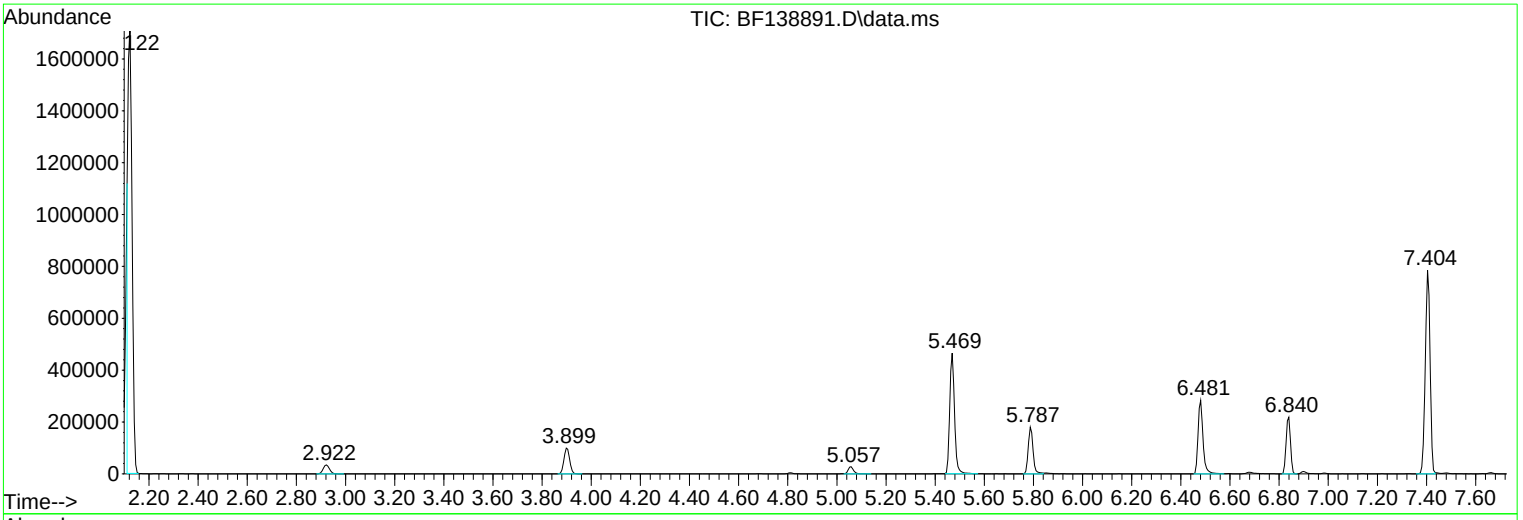
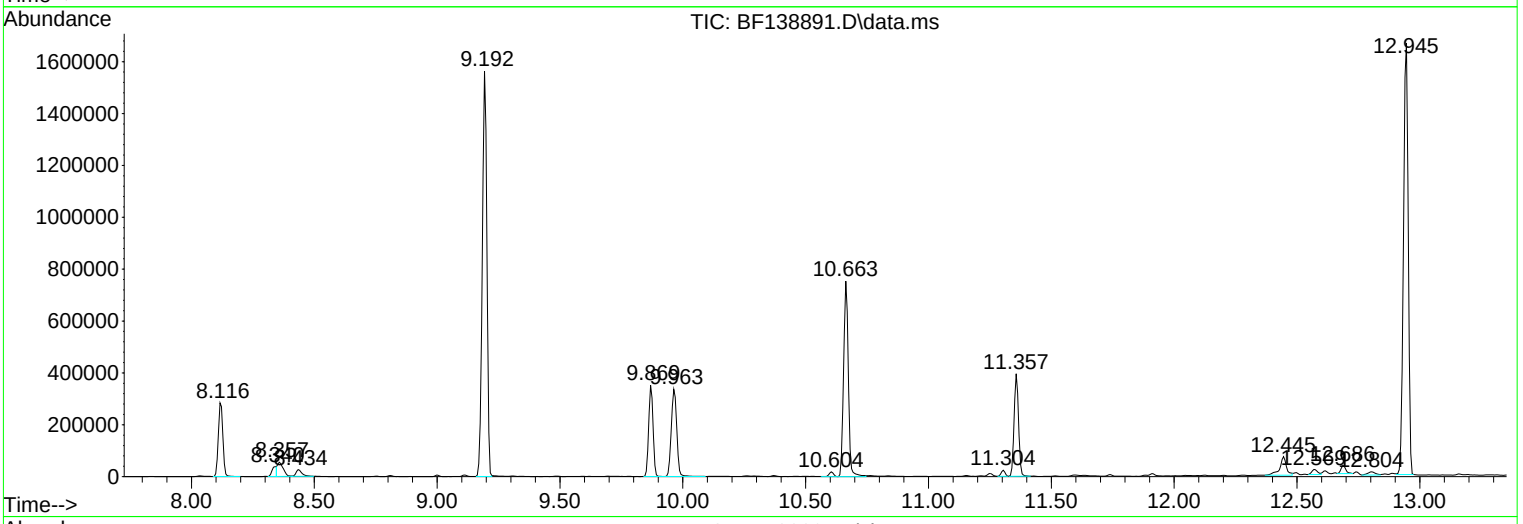
Acq On : 09 Aug 2024 16:33
Operator : RC/JU
Sample : P3469-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

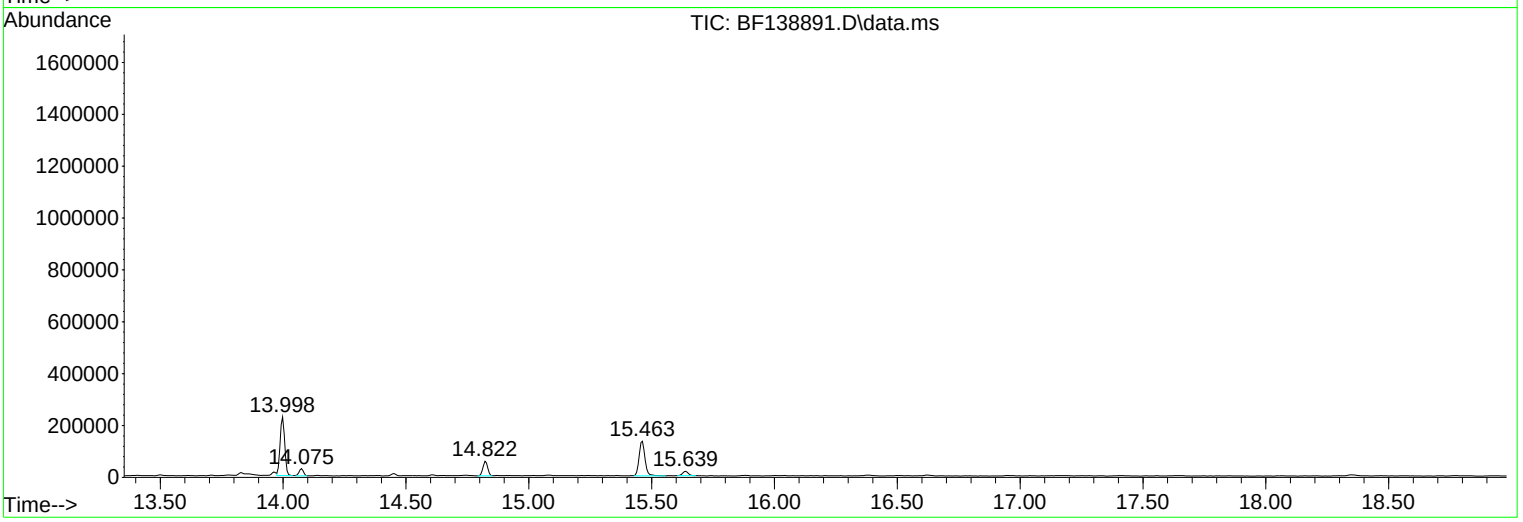
Instrument :
BNA_F
ClientSampleId :
MLS-15-625-640

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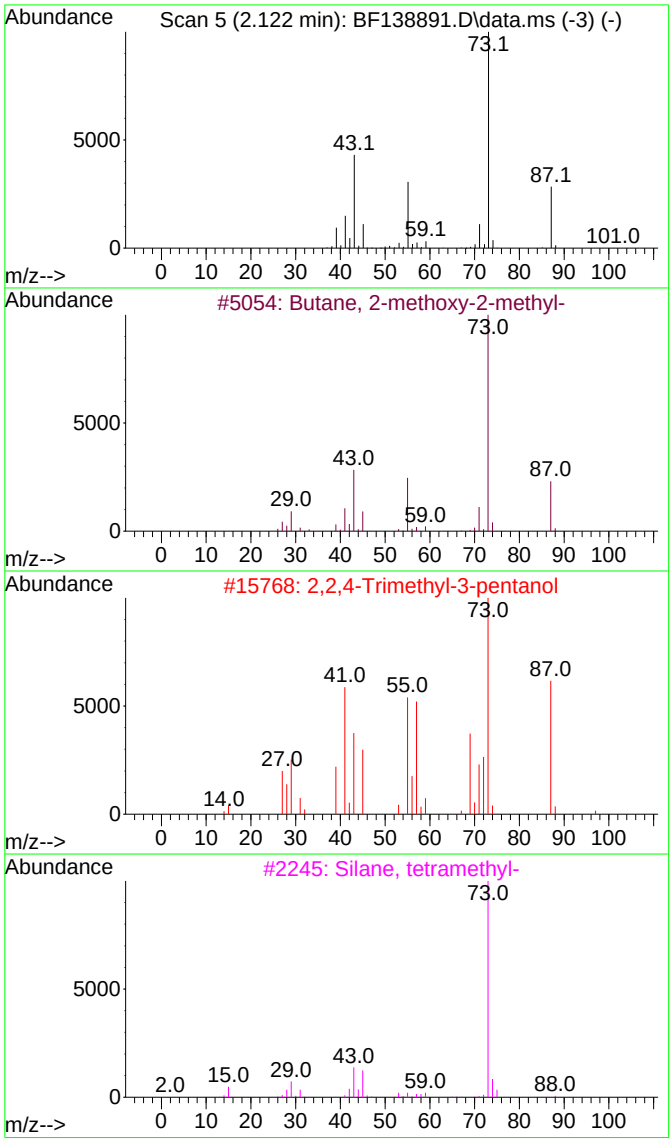
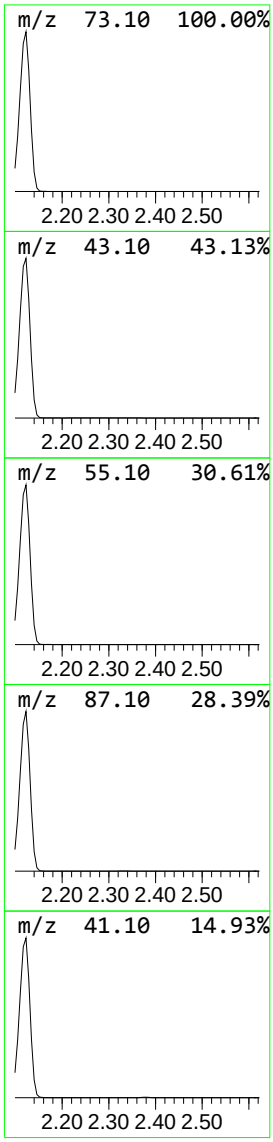
****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.122	142.49 ng	1935100	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	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4	Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	17
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9





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ClientSampleId :
MLS-15-625-640

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

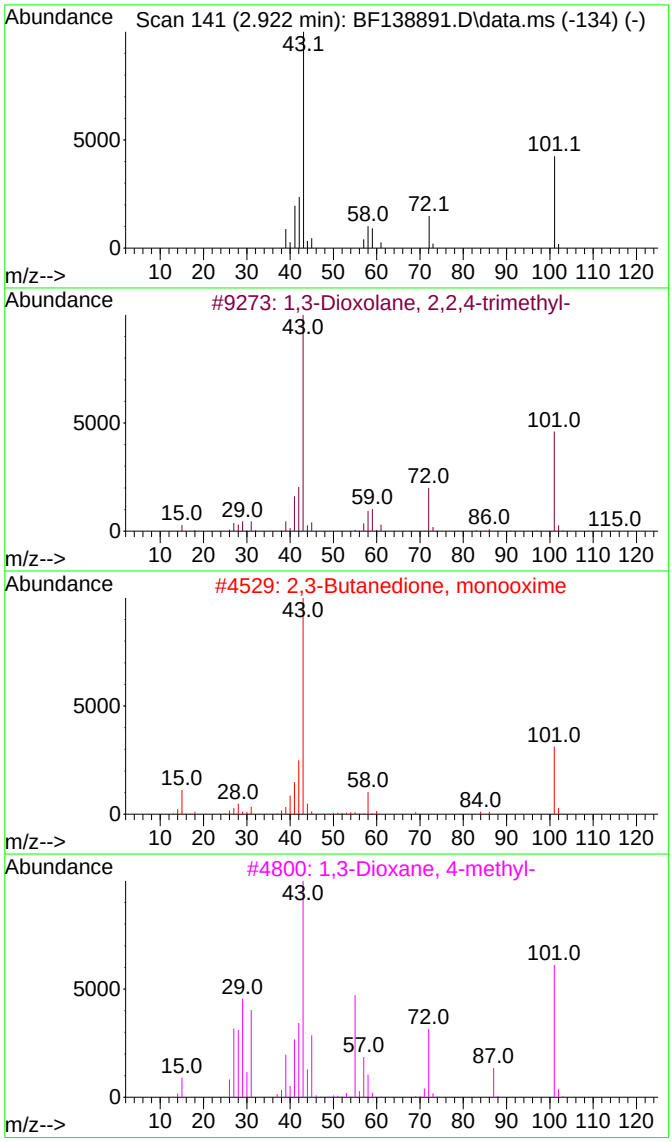
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

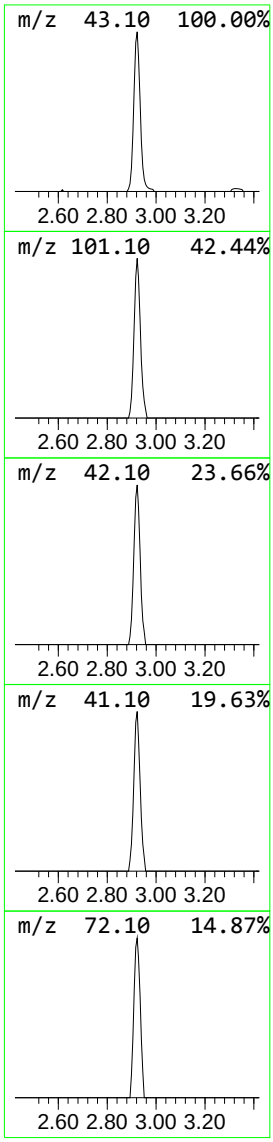
****

Peak Number 2 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.922	4.62 ng	62706	1,4-Dichlorobenzene-d4	6.840

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	78
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	42
3	1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	38
4	1-Methoxy-2-propyl acetate	132	C6H12O3	000108-65-6	12
5	Acetamide, N-(aminocarbonyl)-	102	C3H6N2O2	000591-07-1	9





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ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MLS-15-625-640

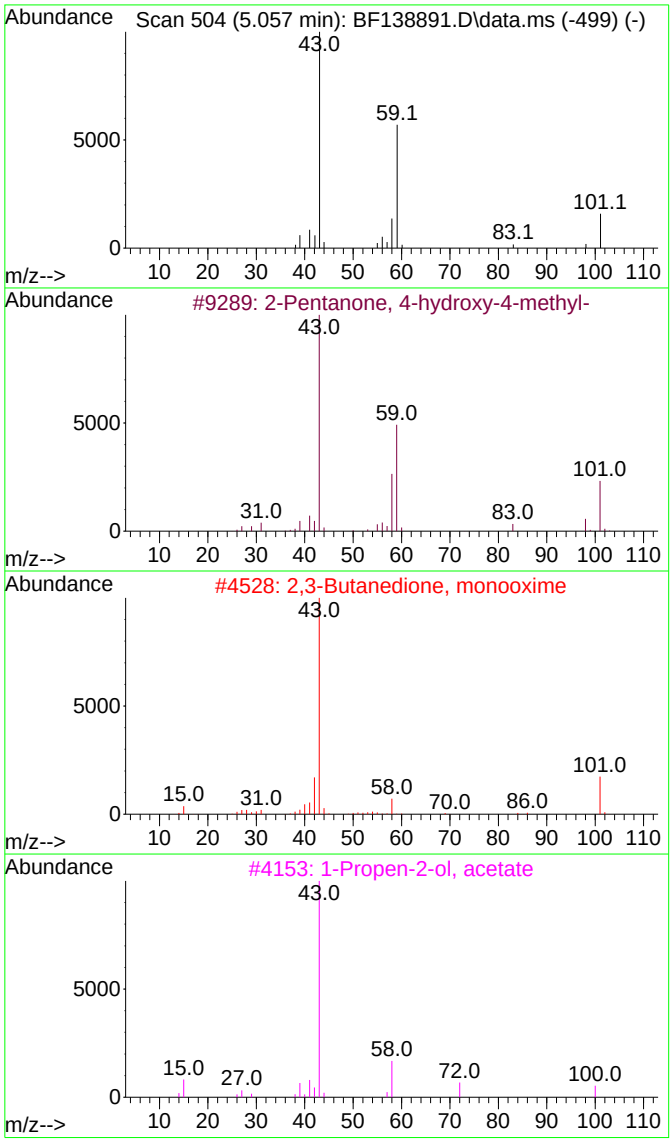
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

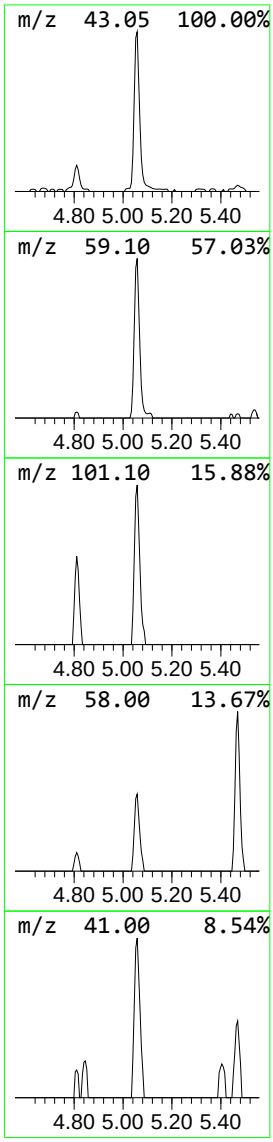
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.057	3.05 ng	41446	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	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080924\
Data File : BF138891.D
Acq On : 09 Aug 2024 16:33
Operator : RC/JU
Sample : P3469-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MLS-15-625-640

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

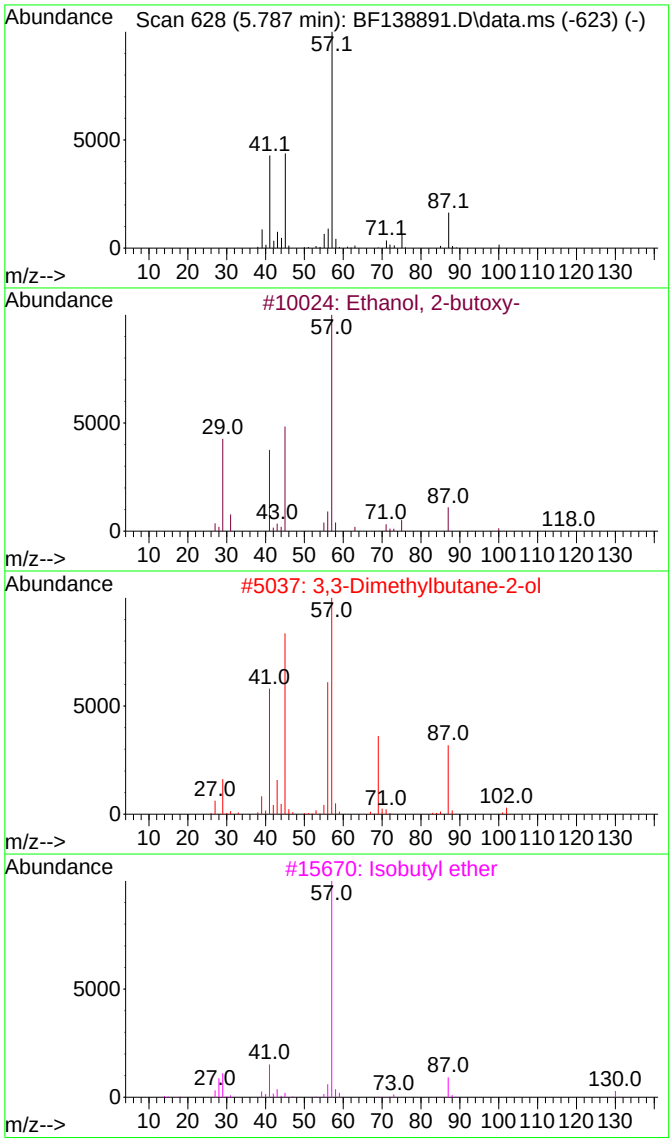
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

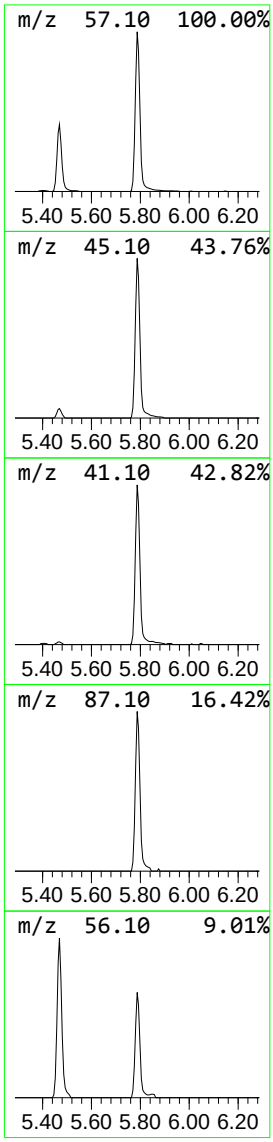
****

Peak Number 5 Ethanol, 2-butoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.787	17.68 ng	240069	1,4-Dichlorobenzene-d4	6.840

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	83
2	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	33
3	Isobutyl ether	130	C8H18O	000628-55-7	25
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	17
5	Propanedioic acid, oxo-, bis(2-m...	230	C11H18O5	092778-43-3	14





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Sample : P3469-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
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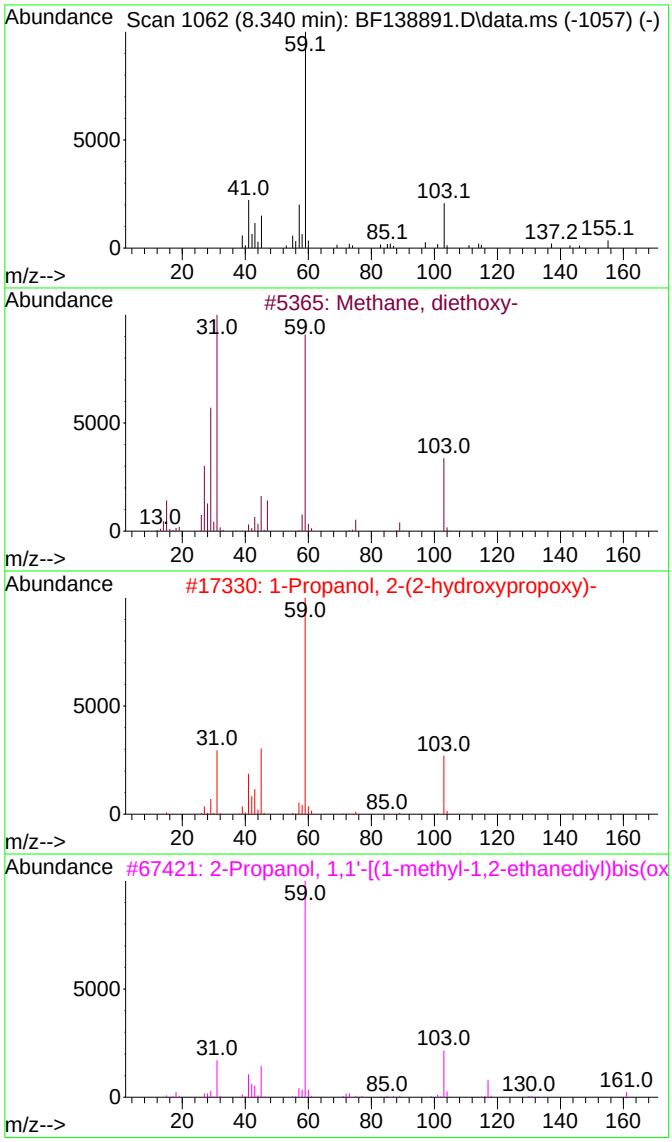
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

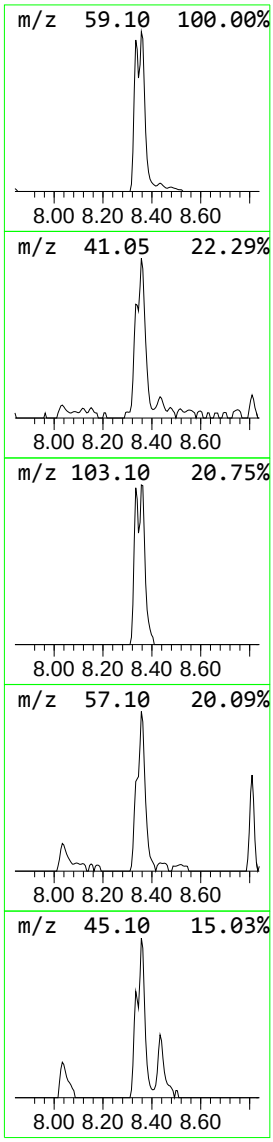
****

Peak Number 6 Methane, diethoxy- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.340	2.78 ng	50762	Naphthalene-d8	8.116

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methane, diethoxy-	104	C5H12O2	000462-95-3	72
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72
3	2-Propanol, 1,1'-[(1-methyl-1,2-...	192	C9H20O4	001638-16-0	72
4	1,4,7-Trimethyl-3,6-dioxaoctane-...	192	C9H20O4	1000423-63-2	64
5	Propane, 1,2-dimethoxy-	104	C5H12O2	007778-85-0	58





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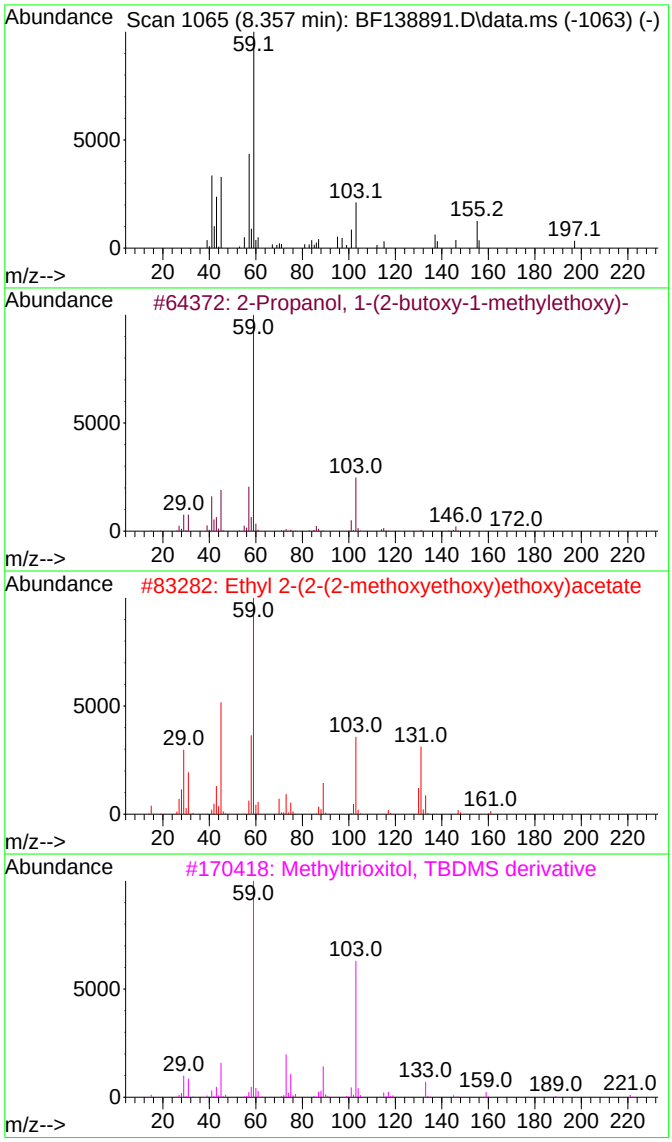
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

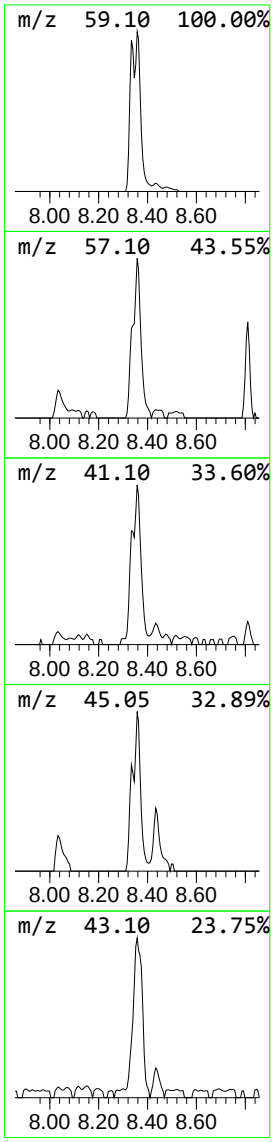
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 2-Propanol, 1-(2-butoxy-1-m... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.357	4.85 ng	88359	Naphthalene-d8	8.116

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	64
2	Ethyl 2-(2-(2-methoxyethoxy)etho...	206	C9H18O5	1000366-89-0	59
3	Methyltrioxitol, TBDMS derivative	278	C13H30O4Si	1000352-09-5	45
4	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	45
5	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	45





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Operator : RC/JU
Sample : P3469-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
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TIC Library : C:\Database\NIST20.L
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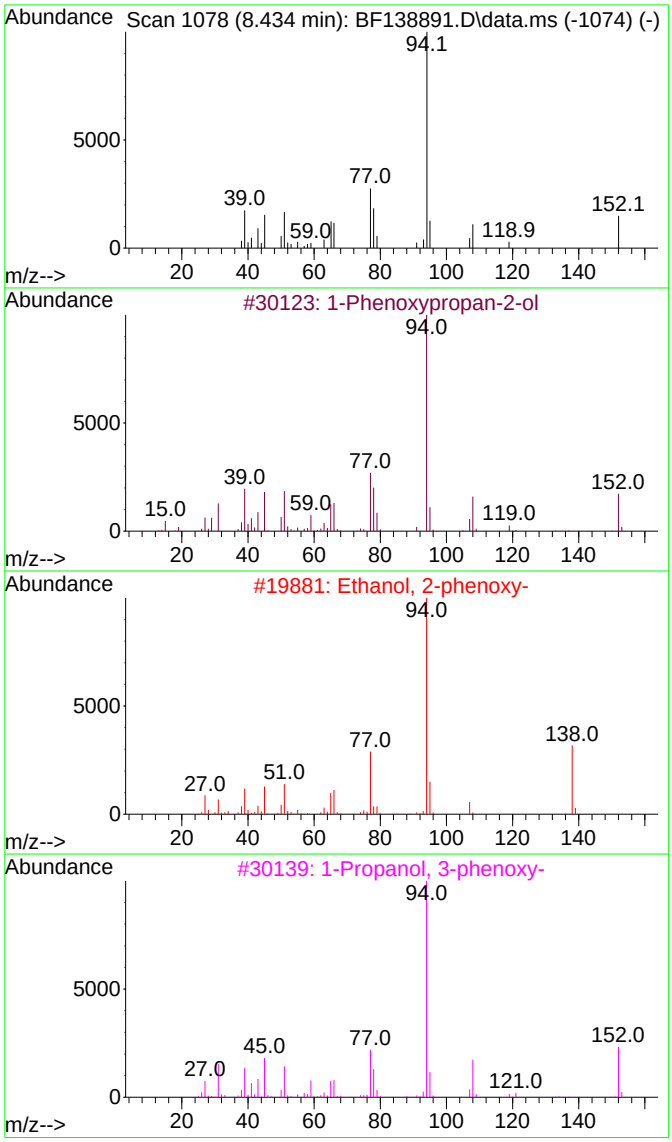
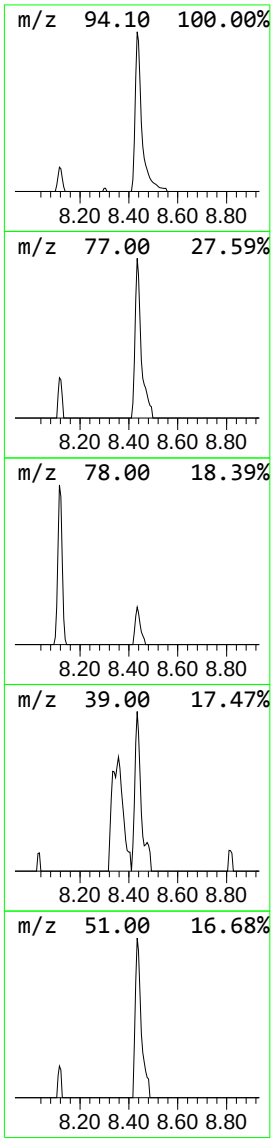
****

Peak Number 8 1-Phenoxypropan-2-ol Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.434	2.34 ng	42699	Naphthalene-d8	8.116

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	94
2	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	72
3	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	72
4	Benzene, (2-methylpropoxy)-	150	C10H14O	001126-75-6	59
5	2-Hexen-4-yne, 2-methyl-	94	C7H10	058275-93-7	59





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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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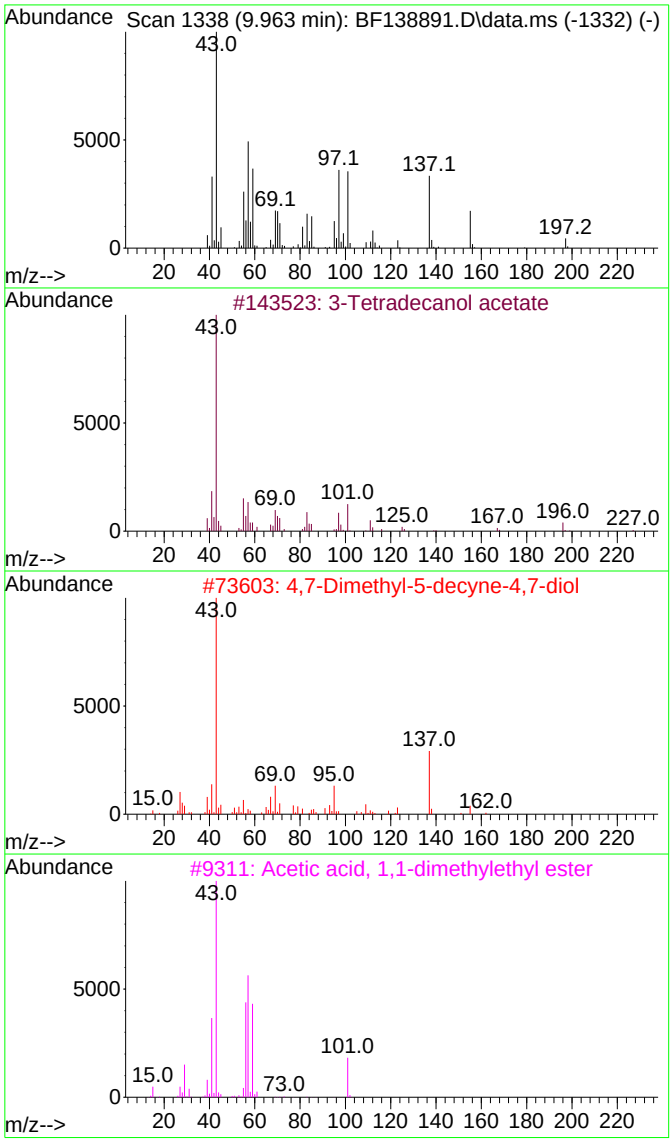
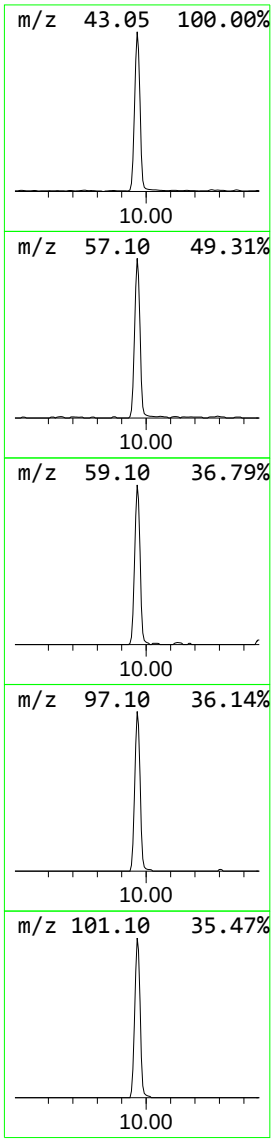
****

Peak Number 9 unknown9.963 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.963	24.05 ng	521651	Acenaphthene-d10	9.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Tetradecanol acetate	256	C16H32O2	051354-23-5	17
2	4,7-Dimethyl-5-decyne-4,7-diol	198	C12H22O2	000126-87-4	12
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	10
4	2-Pentanol, 2-methyl-, acetate	144	C8H16O2	034859-98-8	10
5	3-OXO-4-METHYLPENTANOIC ACID, ME...	144	C7H12O3	042558-54-3	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080924\
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Operator : RC/JU
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Misc :
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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
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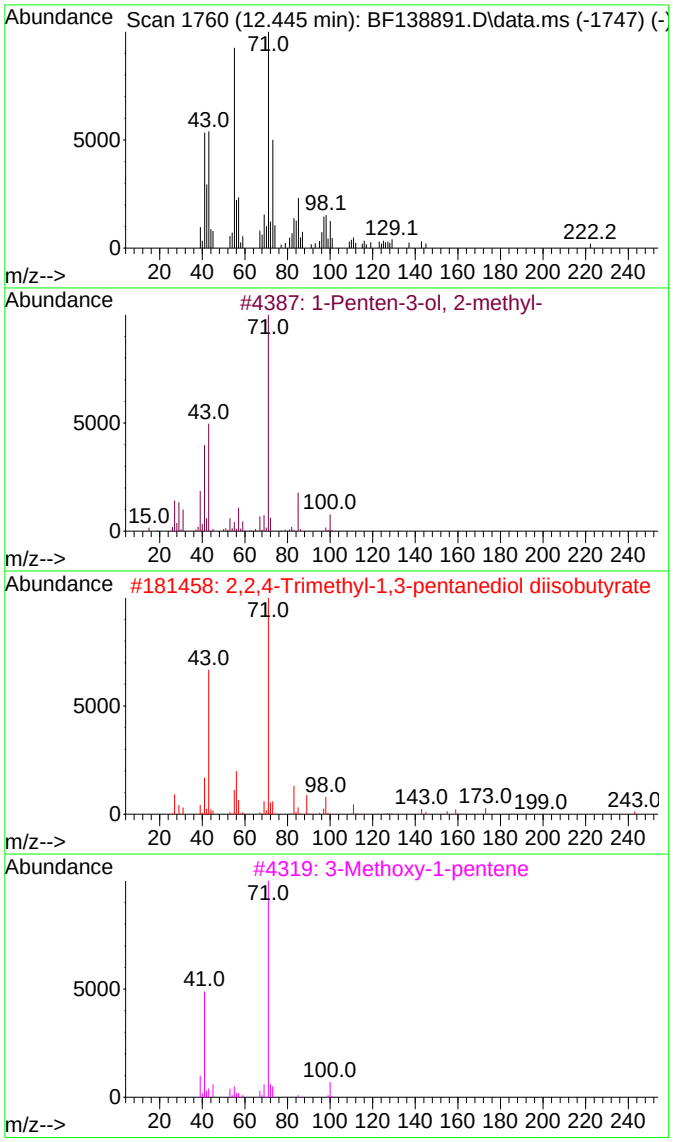
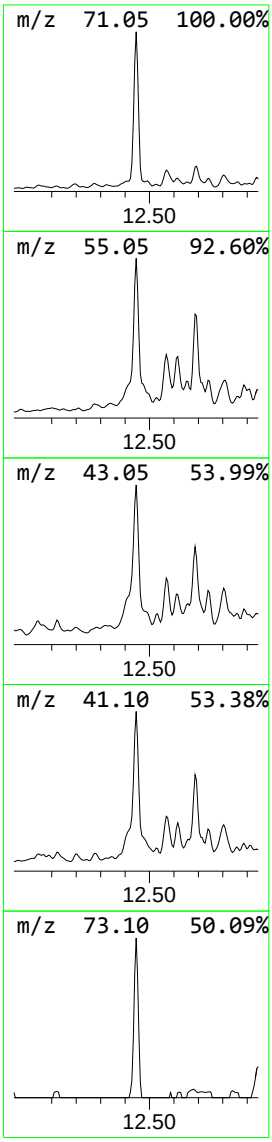
****

Peak Number 10 unknown12.445 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.445	5.55 ng	136685	Phenanthrene-d10	11.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Penten-3-ol, 2-methyl-	100	C6H12O	002088-07-5	49
2	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	47
3	3-Methoxy-1-pentene	100	C6H12O	014092-18-3	43
4	Hexane, 3-methyl-	100	C7H16	000589-34-4	38
5	9-Oxabicyclo[6.1.0]nonane, cis-	126	C8H14O	004925-71-7	30





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Data File : BF138891.D
Acq On : 09 Aug 2024 16:33
Operator : RC/JU
Sample : P3469-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MLS-15-625-640

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

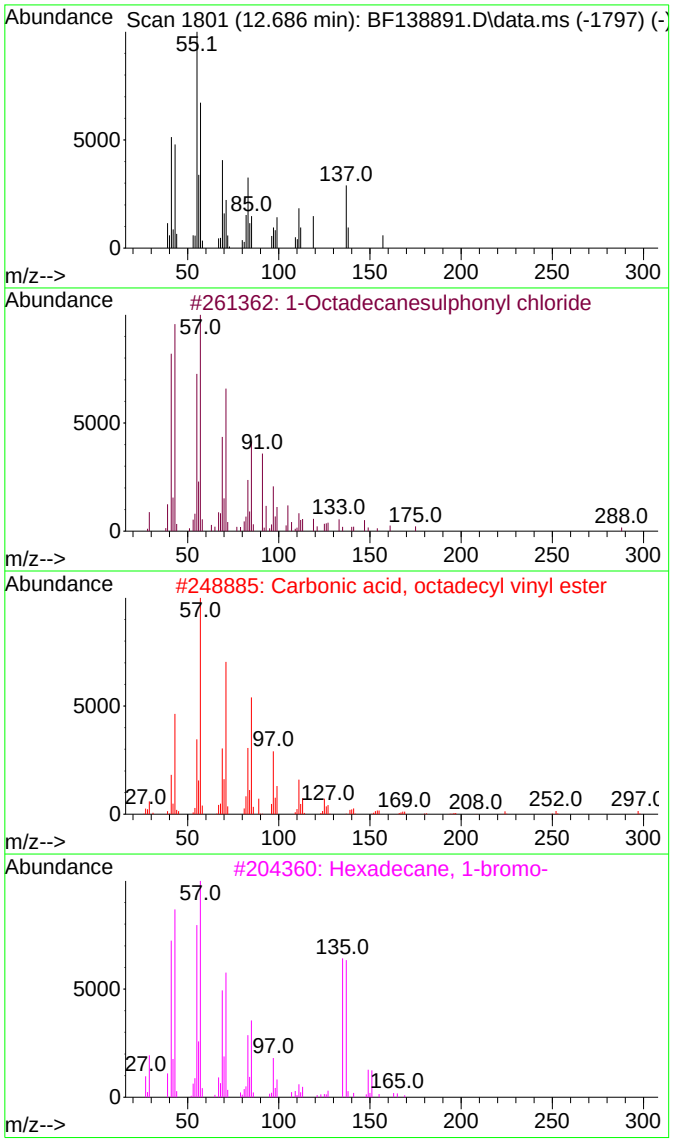
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

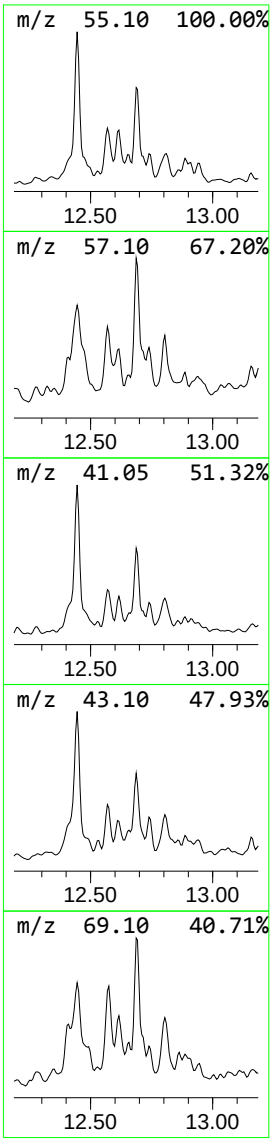
****

Peak Number 11 unknown12.686 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.686	2.95 ng	42160	Chrysene-d12	13.998

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	43
2	Carbonic acid, octadecyl vinyl e...	340	C21H40O3	1000382-54-4	38
3	Hexadecane, 1-bromo-	304	C16H33Br	000112-82-3	38
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	38
5	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080924\
Data File : BF138891.D
Acq On : 09 Aug 2024 16:33
Operator : RC/JU
Sample : P3469-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MLS-15-625-640

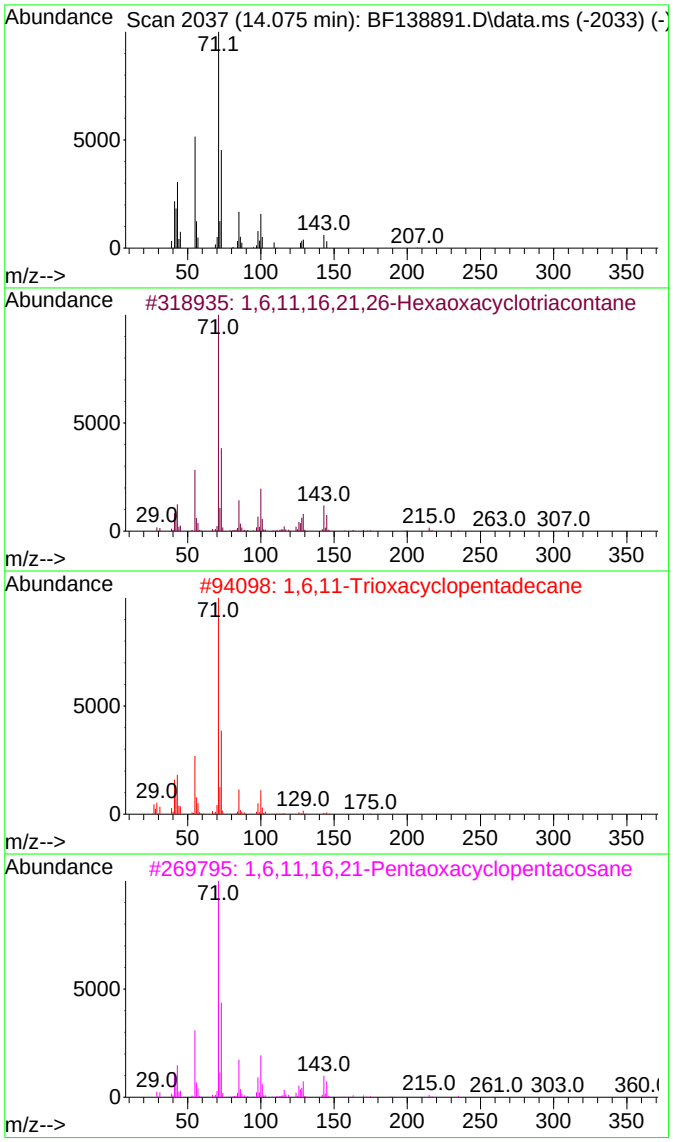
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

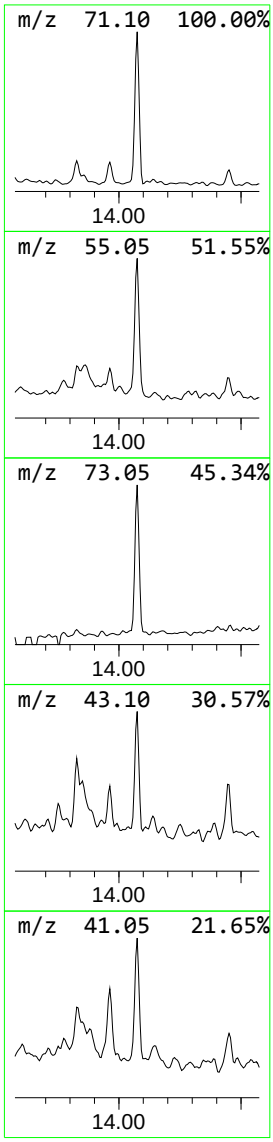
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 1,6,11,16,21,26-Hexaoxacycl... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.075	2.40 ng	34257	Chrysene-d12	13.998

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6,11,16,21,26-Hexaoxacyclotria...	432	C24H48O6	064001-05-4	90
2	1,6,11-Trioxacyclopentadecane	216	C12H24O3	000295-63-6	90
3	1,6,11,16,21-Pentaoxacyclopentac...	360	C20H40O5	056890-57-4	83
4	1,6,11,16-Tetraoxacycloeicosane	288	C16H32O4	017043-02-6	83
5	1,6,11,16,21,26,31-Heptaoxacyclo...	504	C28H56O7	066055-34-3	83





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Data File : BF138891.D
Acq On : 09 Aug 2024 16:33
Operator : RC/JU
Sample : P3469-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MLS-15-625-640

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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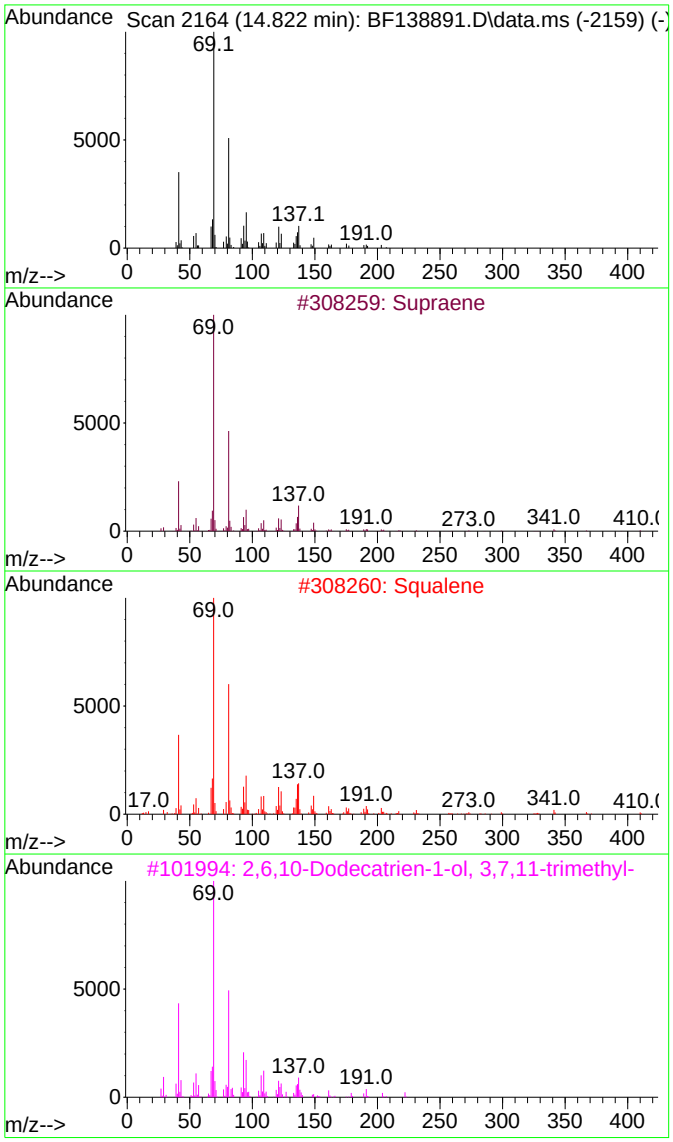
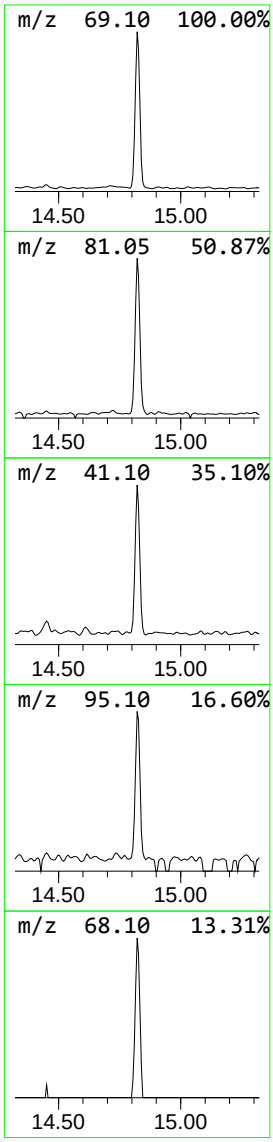
Peak Number 13 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.822	6.73 ng	73991	Perylene-d12	15.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	Squalene	410	C30H50	000111-02-4	91
3	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	78
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5	trans-Farnesol	222	C15H26O	000106-28-5	64





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Acq On : 09 Aug 2024 16:33
Operator : RC/JU
Sample : P3469-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MLS-15-625-640

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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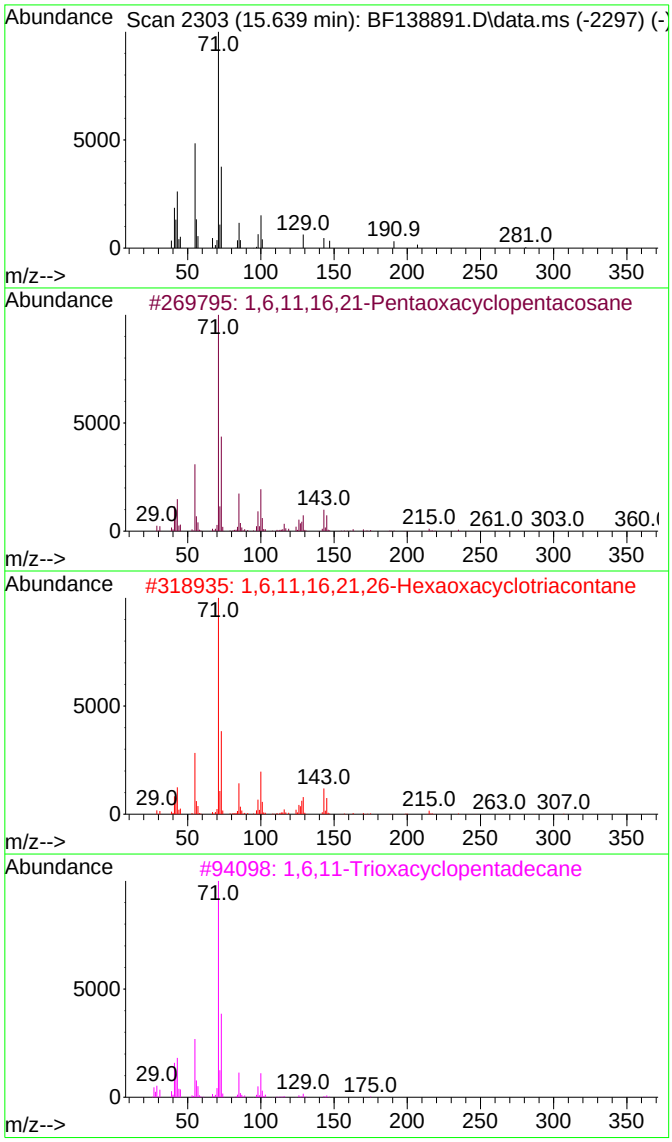
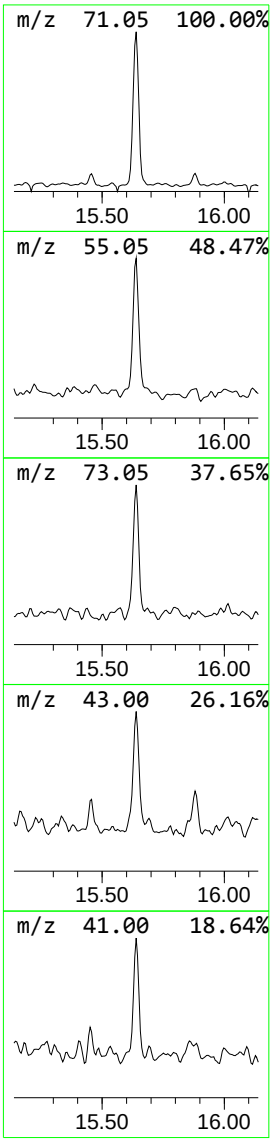
Peak Number 14 1,6,11,16,21-Pentaoxacyclop... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.639	2.47 ng	27132	Perylene-d12	15.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6,11,16,21-Pentaoxacyclopentac...	360	C20H40O5	056890-57-4	83
2	1,6,11,16,21,26-Hexaoxacyclotria...	432	C24H48O6	064001-05-4	83
3	1,6,11-Trioxacyclopentadecane	216	C12H24O3	000295-63-6	78
4	1,6,11,16,21,26,31-Heptaoxacyclo...	504	C28H56O7	066055-34-3	74
5	1,6,11,16-Tetraoxacycloeicosane	288	C16H32O4	017043-02-6	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080924\
Data File : BF138891.D
Acq On : 09 Aug 2024 16:33
Operator : RC/JU
Sample : P3469-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MLS-15-625-640

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	142.5	ng	1935100	1	6.840	271617	20.0
1,3-Dioxolane, ...	2.922	4.6	ng	62706	1	6.840	271617	20.0
2-Pentanone, 4-...	5.057	3.0	ng	41446	1	6.840	271617	20.0
Ethanol, 2-butoxy-	5.787	17.7	ng	240069	1	6.840	271617	20.0
Methane, diethoxy-	8.340	2.8	ng	50762	2	8.116	364728	20.0
2-Propanol, 1-(...	8.357	4.8	ng	88359	2	8.116	364728	20.0
1-Phenoxypropan...	8.434	2.3	ng	42699	2	8.116	364728	20.0
unknown9.963	9.963	24.1	ng	521651	3	9.869	433747	20.0
unknown12.445	12.445	5.5	ng	136685	4	11.357	492313	20.0
unknown12.686	12.686	3.0	ng	42160	5	13.998	285963	20.0
1,6,11,16,21,26...	14.075	2.4	ng	34257	5	13.998	285963	20.0
Supraene	14.822	6.7	ng	73991	6	15.463	219775	20.0
1,6,11,16,21-Pe...	15.639	2.5	ng	27132	6	15.463	219775	20.0