LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080624\
Data File : BF138821.D
Acq On : 06 Aug 2024 22:54
Operator : RC/JU
Sample : P3459-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MLS-15-383-398

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: BF138821.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	6	12	rVB	1675358	2357378	74.17%	14.020%
2	3.904	301	308	319	rBV	395782	637111	20.04%	3.789%
3	5.475	569	575	599	rVB	395001	914209	28.76%	5.437%
4	5.822	623	634	640	rBV	1426699	3178524	100.00%	18.904%
5	6.481	741	746	759	rBV	459979	620188	19.51%	3.688%
6	6.840	802	807	812	rBV	235996	290787	9.15%	1.729%
7	7.404	897	903	908	rBV	754193	1024692	32.24%	6.094%
8	8.116	1019	1024	1032	rBV	311369	396616	12.48%	2.359%
9	8.339	1056	1062	1064	rBV	365188	542433	17.07%	3.226%
10	8.363	1064	1066	1076	rVB	437118	516771	16.26%	3.073%
11	9.192	1201	1207	1212	rBV	1462797	1876645	59.04%	11.161%
12	9.869	1317	1322	1328	rBV	362509	455066	14.32%	2.706%
13	10.663	1451	1457	1472	rBV	829116	1087006	34.20%	6.465%
14	11.357	1570	1575	1583	rBV	381400	466986	14.69%	2.777%
15	12.445	1755	1760	1766	rVB	98418	121879	3.83%	0.725%
16	12.939	1838	1844	1850	rBV	1263723	1700853	53.51%	10.115%
17	13.998	2019	2024	2032	rVB	188006	248152	7.81%	1.476%
18	14.074	2032	2037	2042	rBV	58538	71702	2.26%	0.426%
19	15.457	2266	2272	2285	rVB	154381	236714	7.45%	1.408%
20	15.639	2298	2303	2313	rVB	43433	70712	2.22%	0.421%

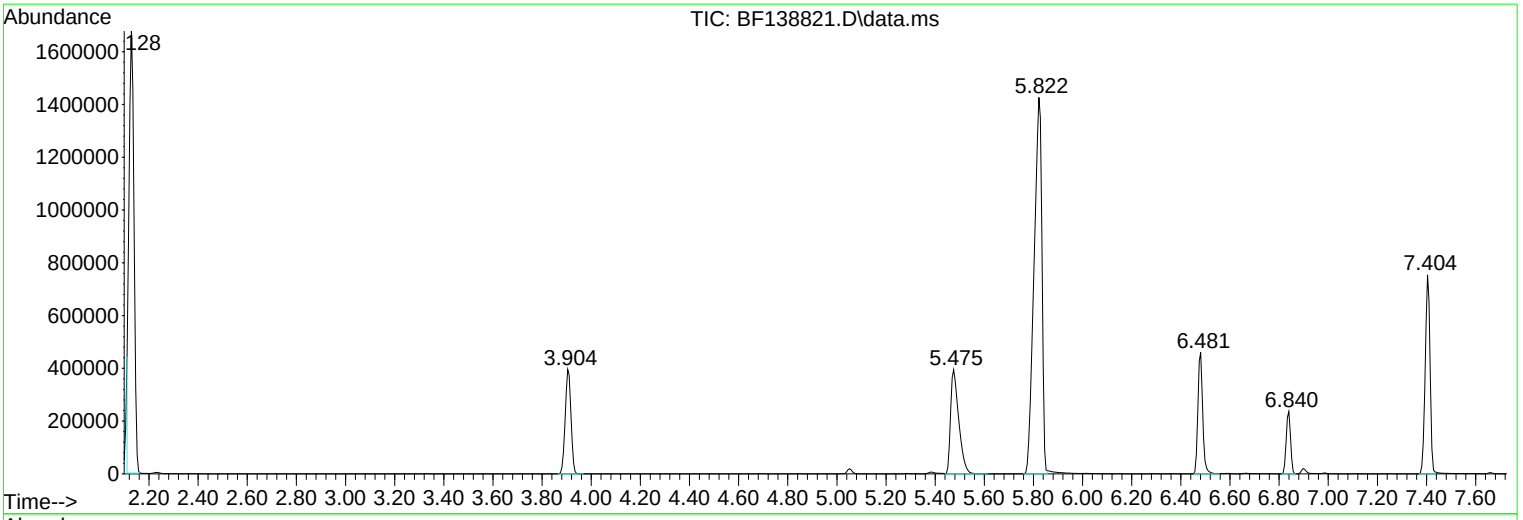
Sum of corrected areas: 16814424

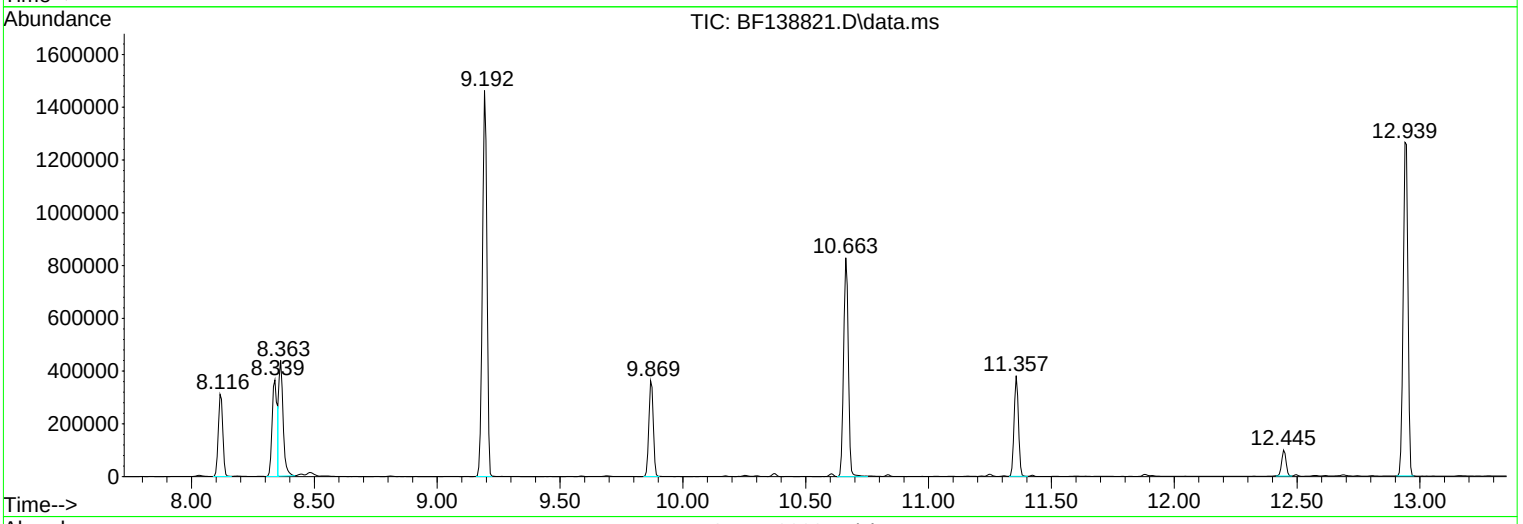
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080624\
Data File : BF138821.D
Acq On : 06 Aug 2024 22:54
Operator : RC/JU
Sample : P3459-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

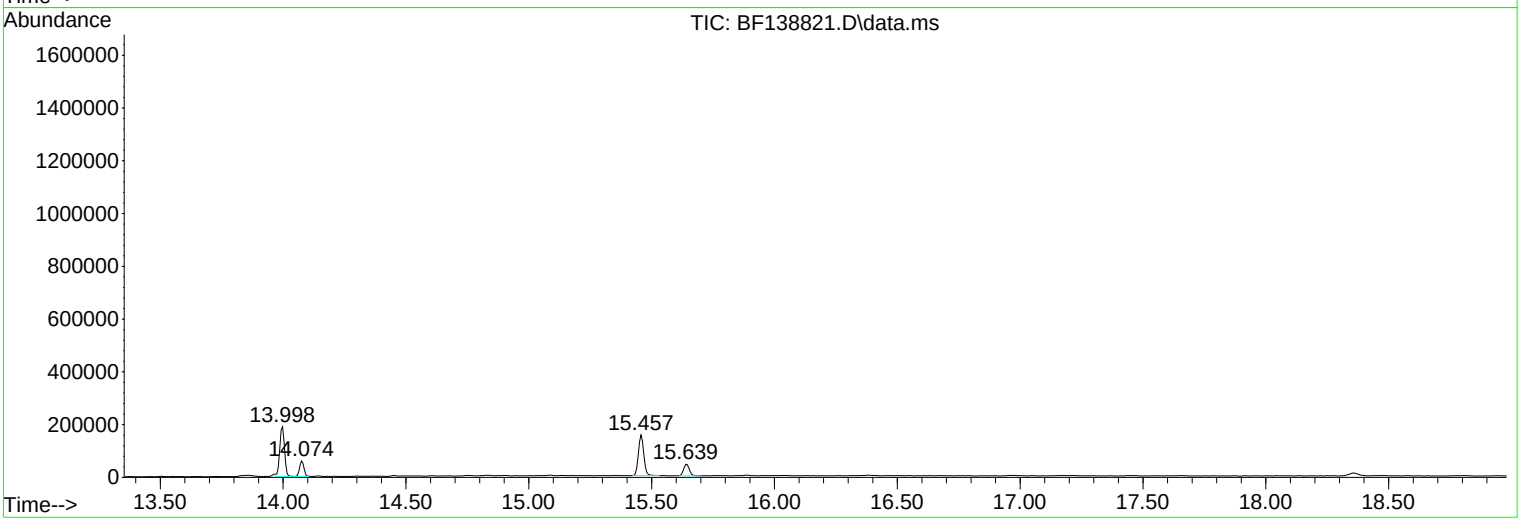
Instrument :
BNA_F
ClientSampleId :
MLS-15-383-398

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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Data File : BF138821.D
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Operator : RC/JU
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

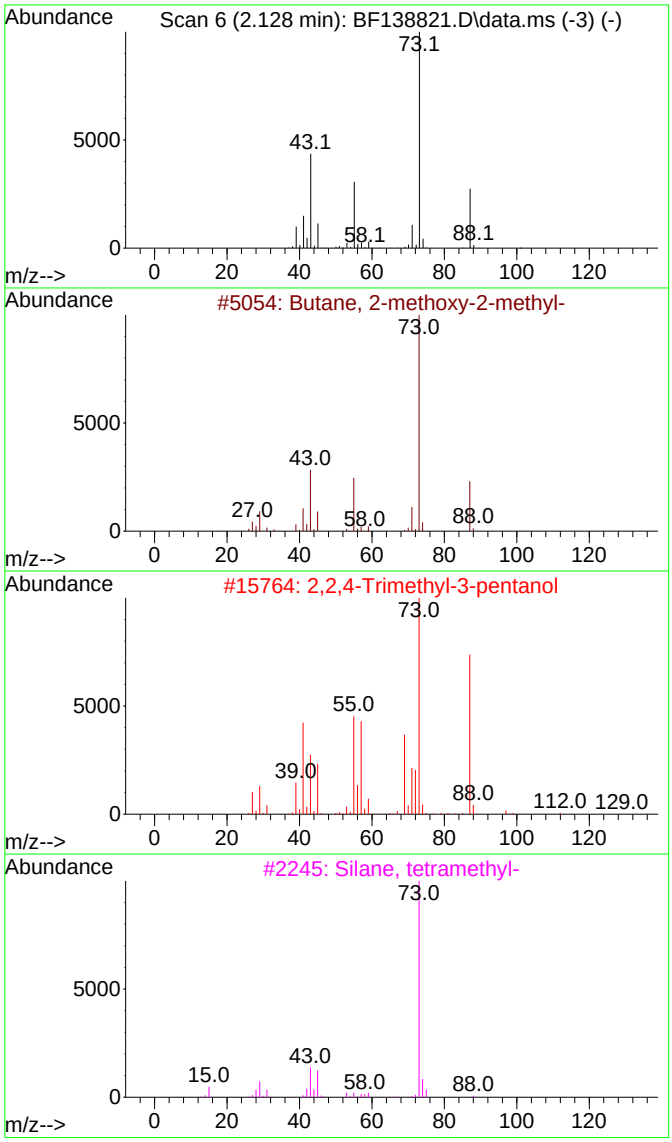
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

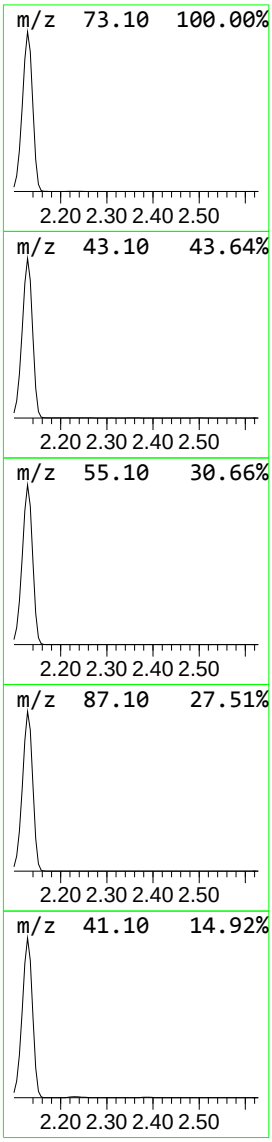
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.128	162.14 ng	2357380	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	Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





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Operator : RC/JU
Sample : P3459-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MLS-15-383-398

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

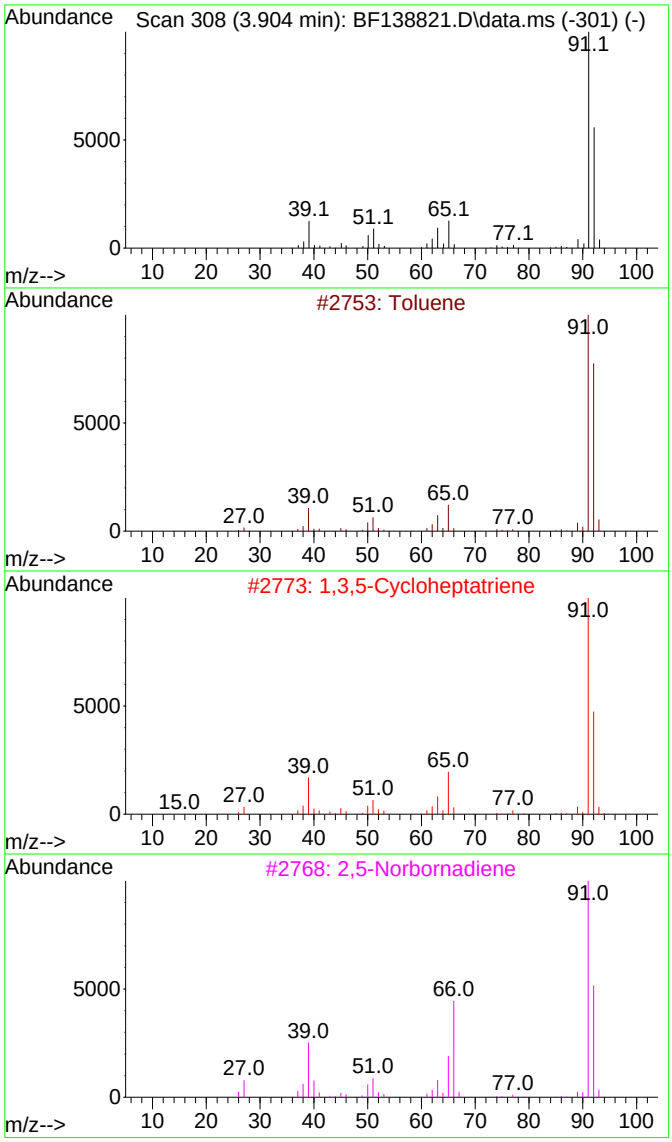
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

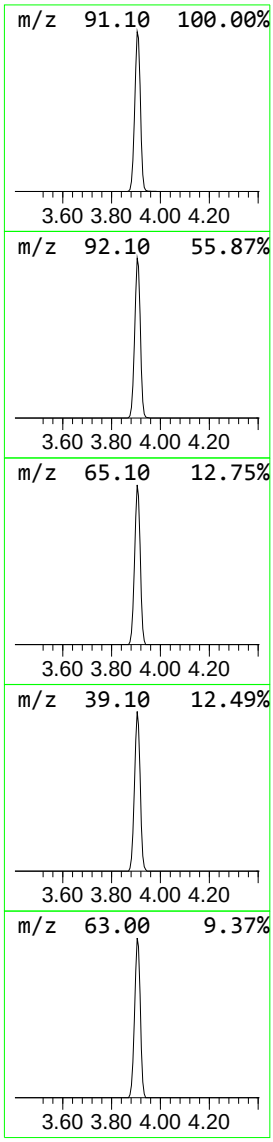
****

Peak Number 2 Toluene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.904	43.82 ng	637111	1,4-Dichlorobenzene-d4	6.840

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Toluene	92	C7H8	000108-88-3	95
2	1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	90
3	2,5-Norbornadiene	92	C7H8	000121-46-0	87
4	Cyclobutene, 2-propenylidene-	92	C7H8	052097-85-5	80
5	Molybdenum, di-.mu.-chlorobis[(1...	532	C20H26Cl2Mo2	035625-66-2	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080624\
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Operator : RC/JU
Sample : P3459-03
Misc :
ALS Vial : 11 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

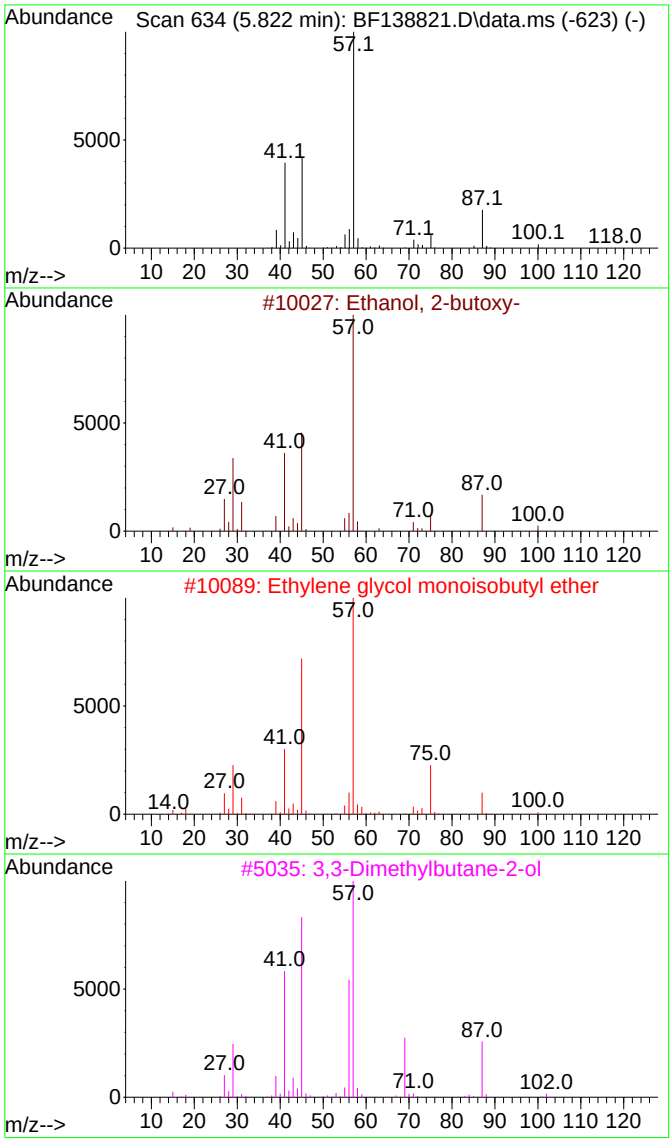
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

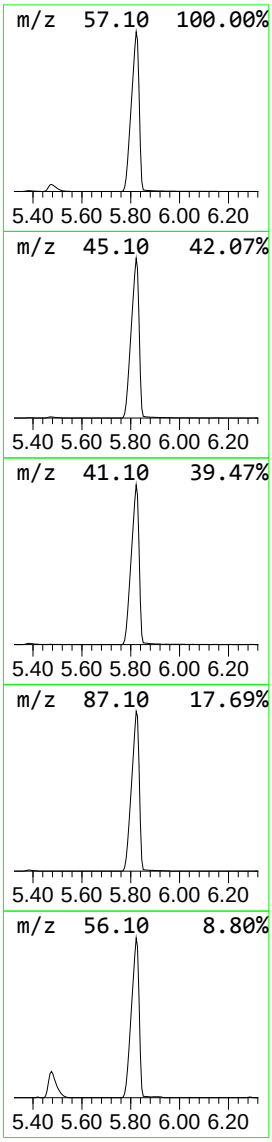
****

Peak Number 3 Ethanol, 2-butoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.822	218.62 ng	3178520	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	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
3	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	42
4	n-Butyl ether	130	C8H18O	000142-96-1	16
5	1-Butene, 4-butoxy-	128	C8H16O	034061-76-2	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080624\
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Operator : RC/JU
Sample : P3459-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MLS-15-383-398

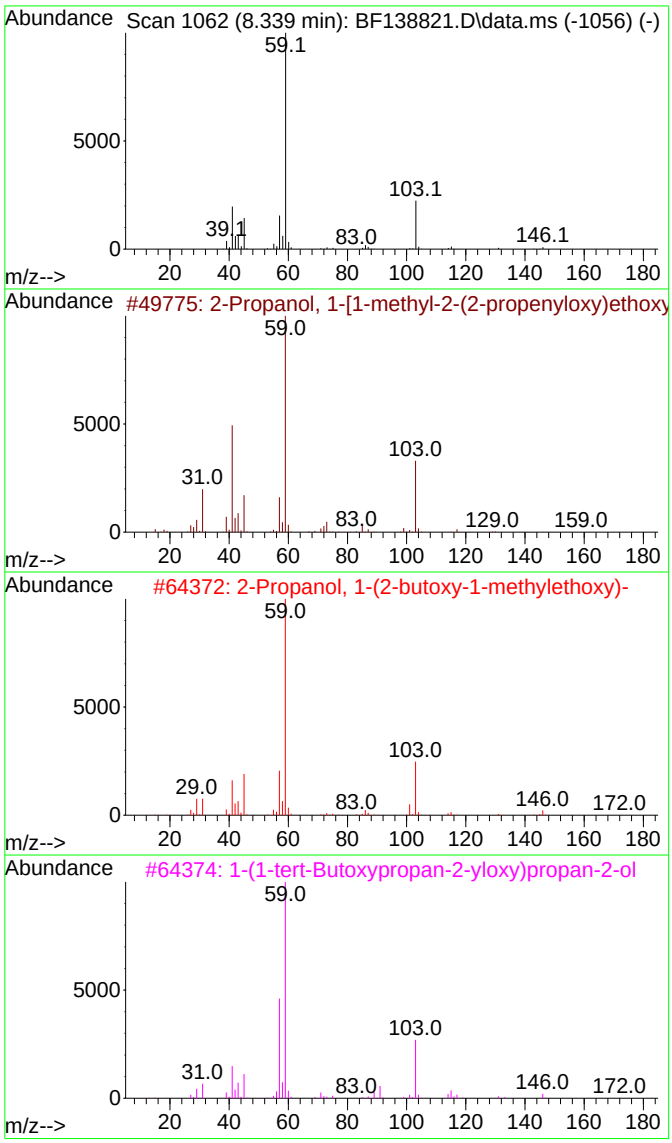
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

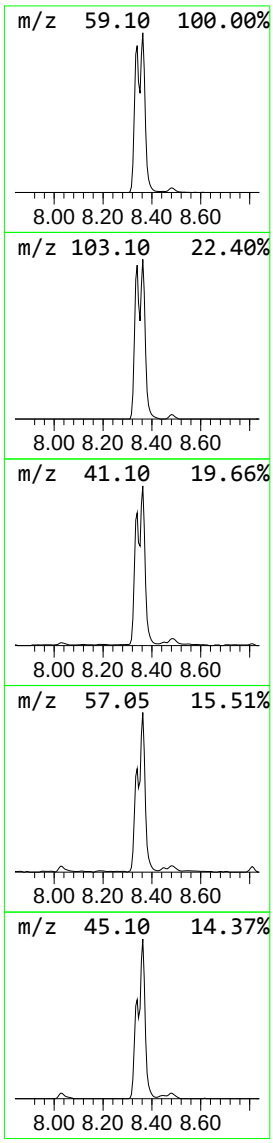
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Propanol, 1-[1-methyl-2-(... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.339	27.35 ng	542433	Naphthalene-d8	8.116

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	83
2	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	83
3	1-(1-tert-Butoxypropan-2-yloxy)p...	190	C10H22O3	132739-31-2	72
4	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72
5	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	64





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Operator : RC/JU
Sample : P3459-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MLS-15-383-398

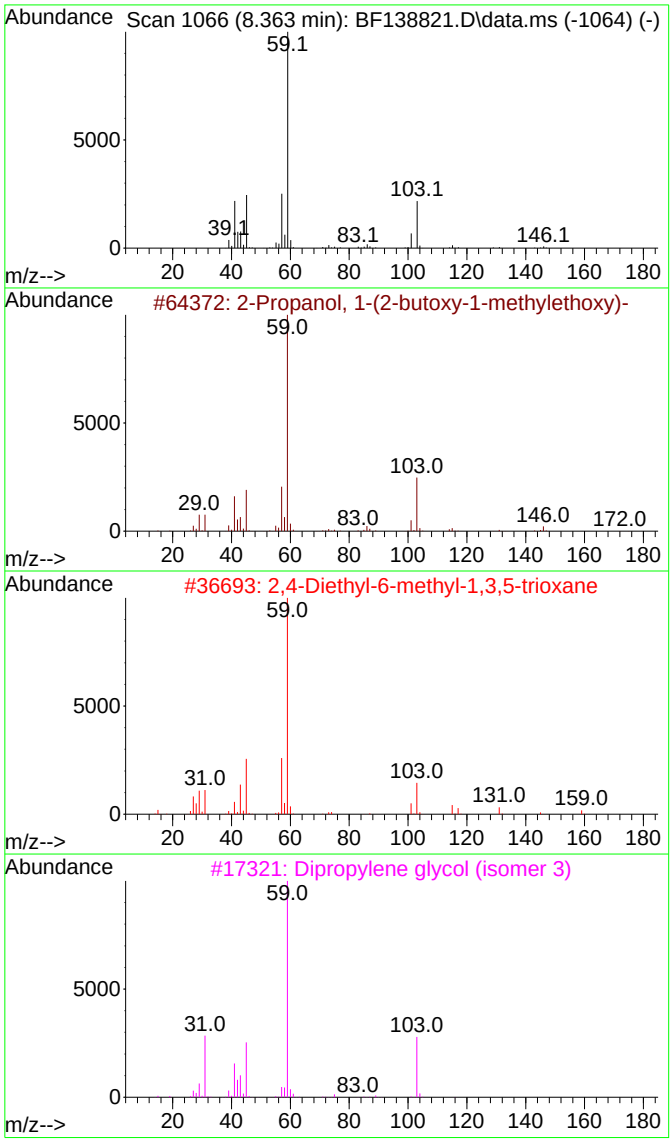
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

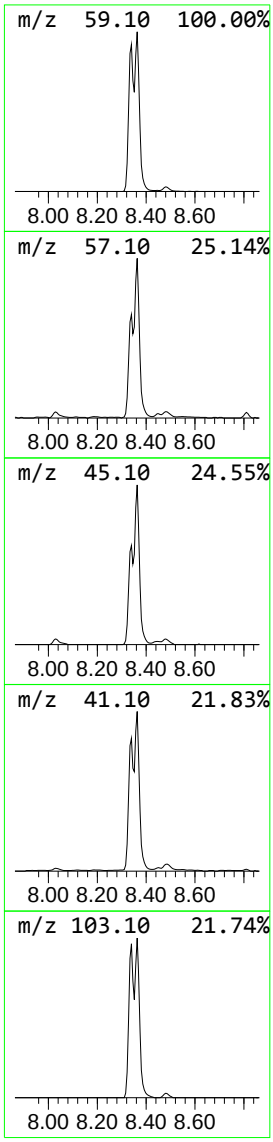
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Propanol, 1-(2-butoxy-1-m... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.363	26.06 ng	516771	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	78
2	2,4-Diethyl-6-methyl-1,3,5-trioxane	160	C8H16O3	117888-04-7	78
3	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	72
4	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	72
5	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	72





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

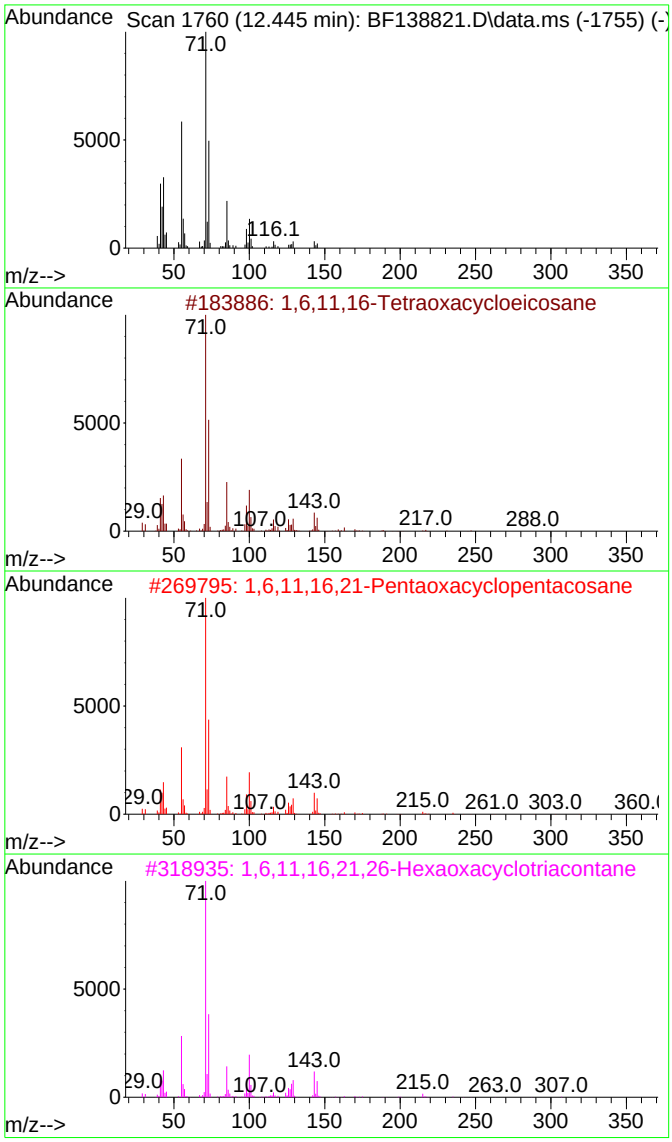
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

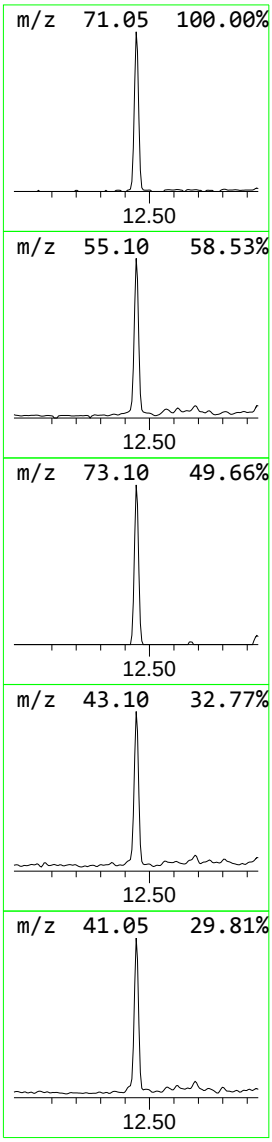
****

Peak Number 6 1,6,11,16-Tetraoxacycloeico... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.445	5.22 ng	121879	Phenanthrene-d10	11.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6,11,16-Tetraoxacycloeicosane	288	C16H32O4	017043-02-6	90
2	1,6,11,16,21-Pentaoxacyclopentac...	360	C20H40O5	056890-57-4	72
3	1,6,11,16,21,26-Hexaoxacyclotria...	432	C24H48O6	064001-05-4	64
4	4-Heptanone, 3-methyl-	128	C8H16O	015726-15-5	59
5	1,6,11-Trioxacyclopentadecane	216	C12H24O3	000295-63-6	53





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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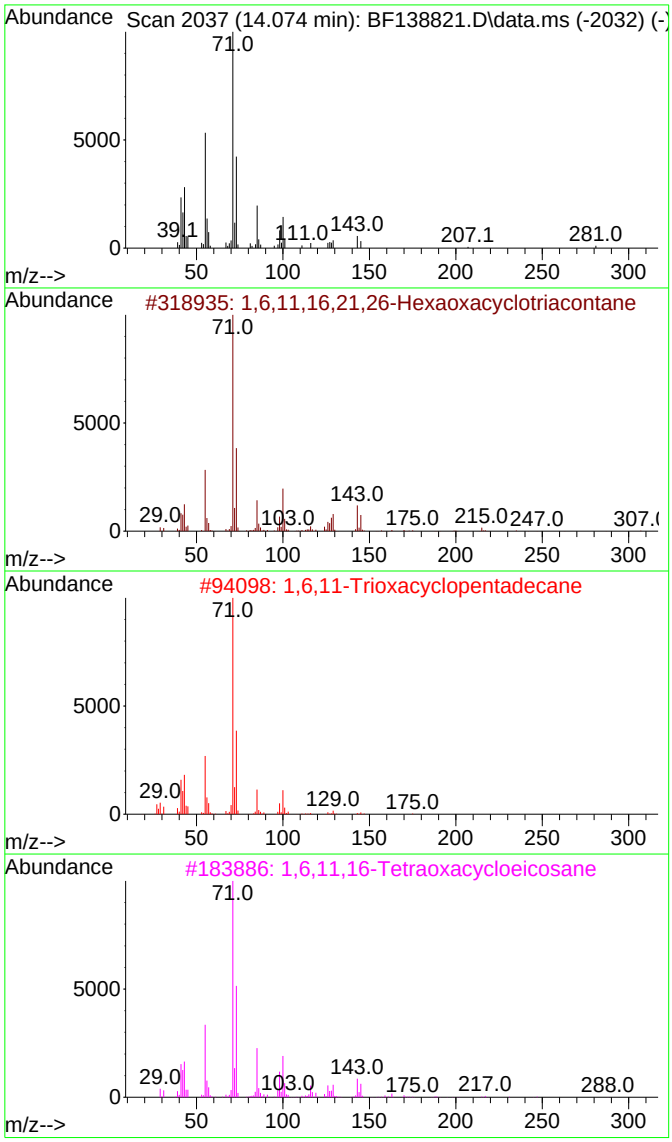
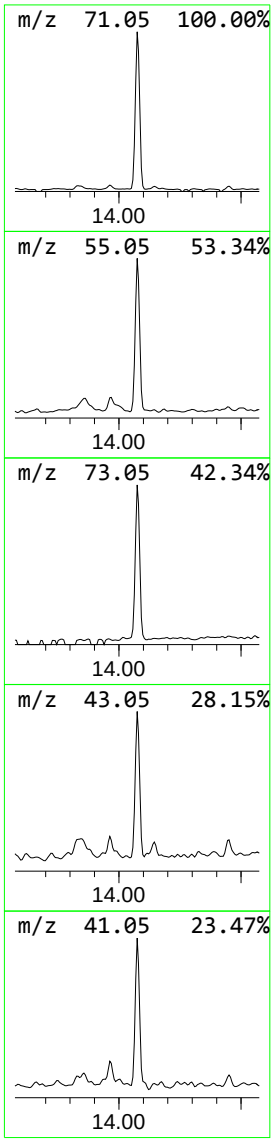
****

Peak Number 7 1,6,11,16,21,26-Hexaoxacycl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.074	5.78 ng	71702	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	86
3	1,6,11,16-Tetraoxacycloeicosane	288	C16H32O4	017043-02-6	83
4	1,6,11,16,21-Pentaoxacyclopentac...	360	C20H40O5	056890-57-4	78
5	1-Penten-3-ol, 2-methyl-	100	C6H12O	002088-07-5	64





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TIC Integration Parameters: LSCINT.P

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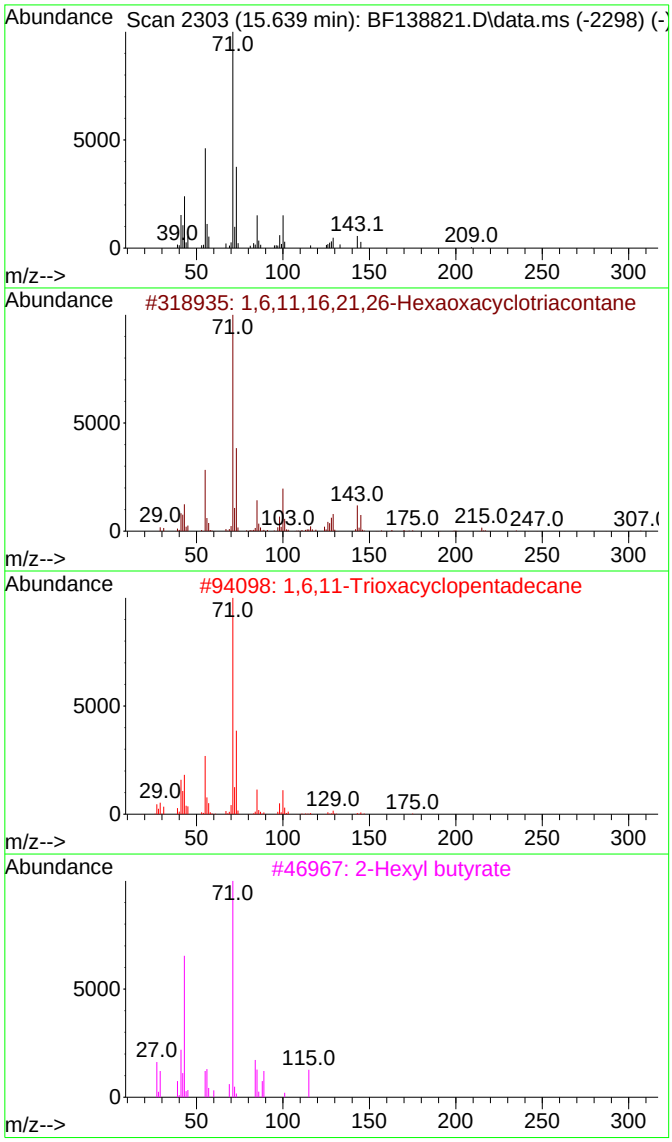
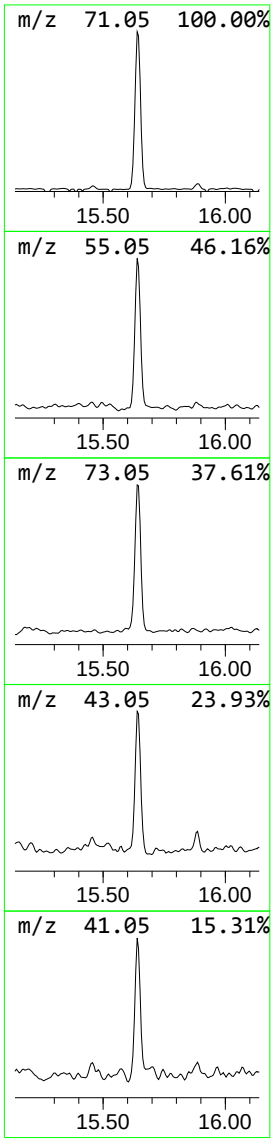
Peak Number 8 1,6,11-Trioxacyclopentadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.639	5.97 ng	70712	Perylene-d12	15.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6,11,16,21,26-Hexaoxacyclotria...	432	C24H48O6	064001-05-4	91
2	1,6,11-Trioxacyclopentadecane	216	C12H24O3	000295-63-6	86
3	2-Hexyl butyrate	172	C10H20O2	1000428-84-6	53
4	3-Methoxybut-1-ene	86	C5H10O	017351-24-5	50
5	Butanoic acid, 2-butoxy-1-methyl...	216	C11H20O4	007492-70-8	50





Tentatively Identified Compound (LSC) summary

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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...	2.128	162.1	ng	2357380	1	6.840	290787	20.0
Toluene	3.904	43.8	ng	637111	1	6.840	290787	20.0
Ethanol, 2-butoxy-	5.822	218.6	ng	3178520	1	6.840	290787	20.0
2-Propanol, 1-[...	8.339	27.4	ng	542433	2	8.116	396616	20.0
2-Propanol, 1-(...	8.363	26.1	ng	516771	2	8.116	396616	20.0
1,6,11,16-Tetra...	12.445	5.2	ng	121879	4	11.357	466986	20.0
1,6,11,16,21,26...	14.074	5.8	ng	71702	5	13.998	248152	20.0
1,6,11-Trioxacy...	15.639	6.0	ng	70712	6	15.457	236714	20.0