LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062024\
Data File : BF138273.D
Acq On : 20 Jun 2024 20:43
Operator : CG\JU
Sample : P2977-16
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OSTL-C4

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-BF061224.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138273.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	10	16	21	rVB	2399390	2937557	57.37%	6.952%
2	3.404	218	224	233	rBV	206584	438857	8.57%	1.039%
3	5.098	509	512	520	rVB	250304	261343	5.10%	0.618%
4	5.504	576	581	584	rBV	4446550	3986024	77.85%	9.433%
5	6.510	747	752	755	rBV	4116202	4013544	78.39%	9.498%
6	6.704	782	785	800	rBV	291911	286112	5.59%	0.677%
7	6.881	812	815	819	rVB	1946200	1605345	31.35%	3.799%
8	7.445	906	911	914	rBV	2728992	2559381	49.99%	6.057%
9	7.698	950	954	958	rBV	158593	140647	2.75%	0.333%
10	8.163	1029	1033	1037	rBV	2680893	2149301	41.98%	5.086%
11	8.381	1065	1070	1078	rBV	73525	66758	1.30%	0.158%
12	8.475	1082	1086	1104	rBV	392023	448367	8.76%	1.061%
13	9.239	1211	1216	1219	rBV	6316829	5120097	100.00%	12.117%
14	9.916	1328	1331	1335	rBV	2787945	2490734	48.65%	5.894%
15	10.016	1343	1348	1357	rBV	1217964	1622551	31.69%	3.840%
16	10.704	1461	1465	1482	rBV	3683368	3247443	63.43%	7.685%
17	11.404	1580	1584	1587	rBV	2972535	2432886	47.52%	5.758%
18	11.792	1647	1650	1654	rVB	73511	62668	1.22%	0.148%
19	11.927	1669	1673	1682	rBV	232894	240972	4.71%	0.570%
20	12.504	1765	1771	1779	rVB2	118631	133766	2.61%	0.317%
21	12.986	1849	1853	1857	rBV	5266076	4615785	90.15%	10.923%
22	14.039	2028	2032	2040	rVB	1718175	1449141	28.30%	3.429%
23	14.898	2174	2178	2182	rBV	68446	63393	1.24%	0.150%
24	15.510	2277	2282	2296	rBV	1207656	1571513	30.69%	3.719%
25	17.180	2559	2566	2574	rVB3	157900	311495	6.08%	0.737%

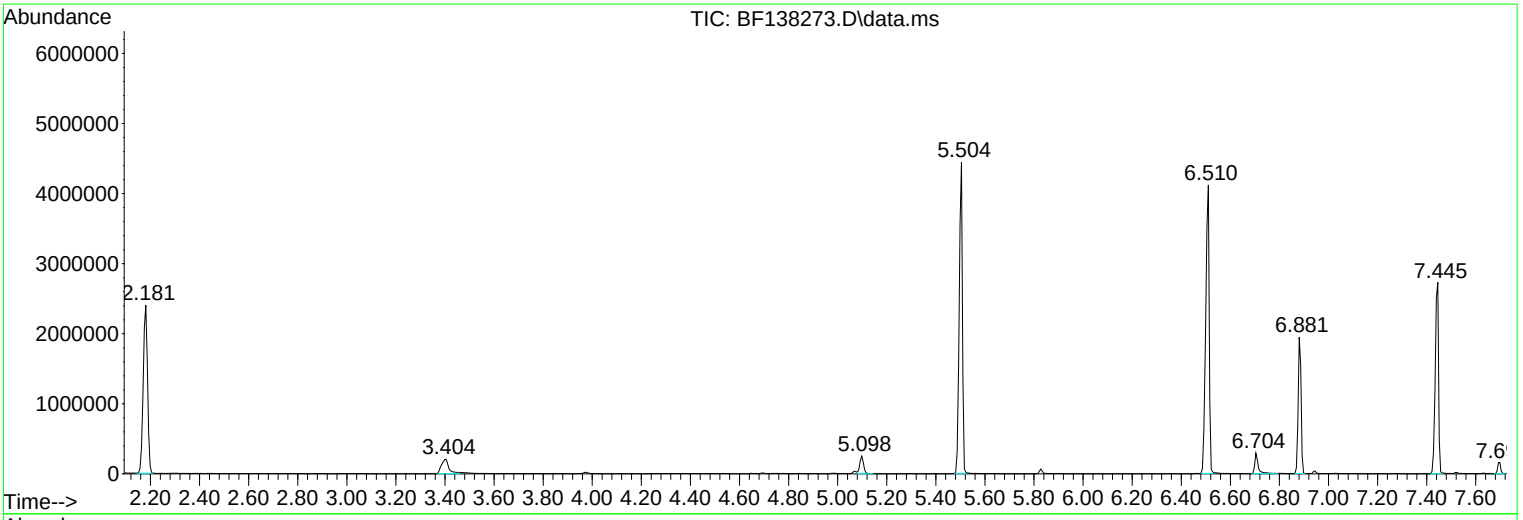
Sum of corrected areas: 42255680

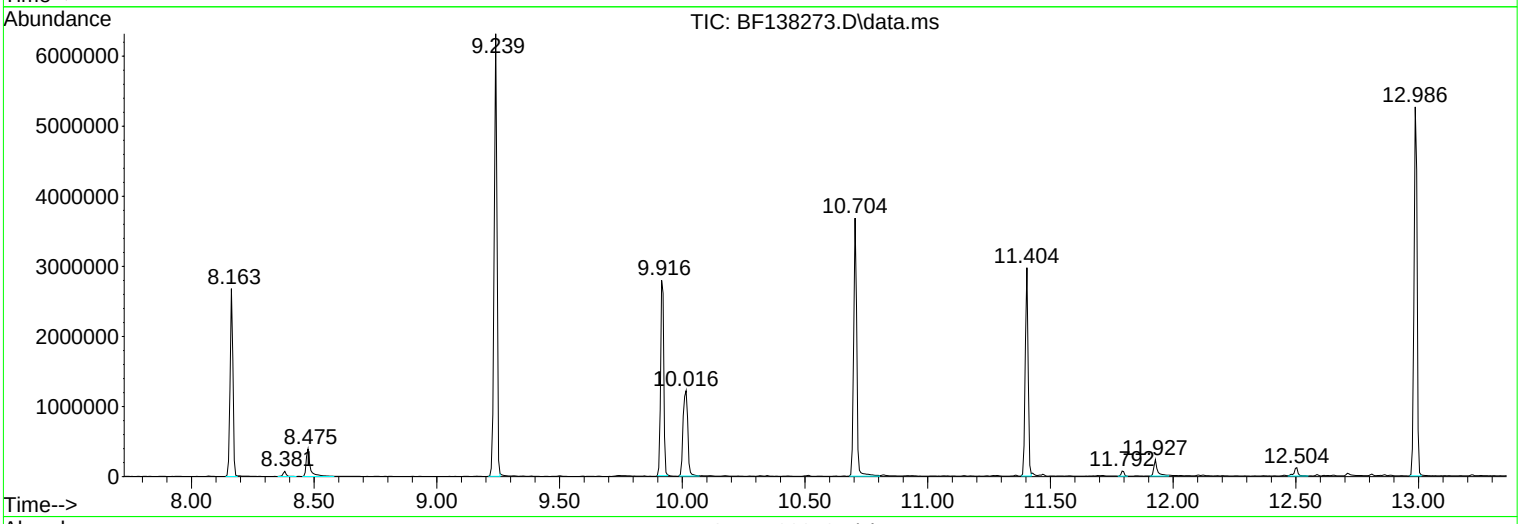
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062024\
Data File : BF138273.D
Acq On : 20 Jun 2024 20:43
Operator : CG\JU
Sample : P2977-16
Misc :
ALS Vial : 16 Sample Multiplier: 1

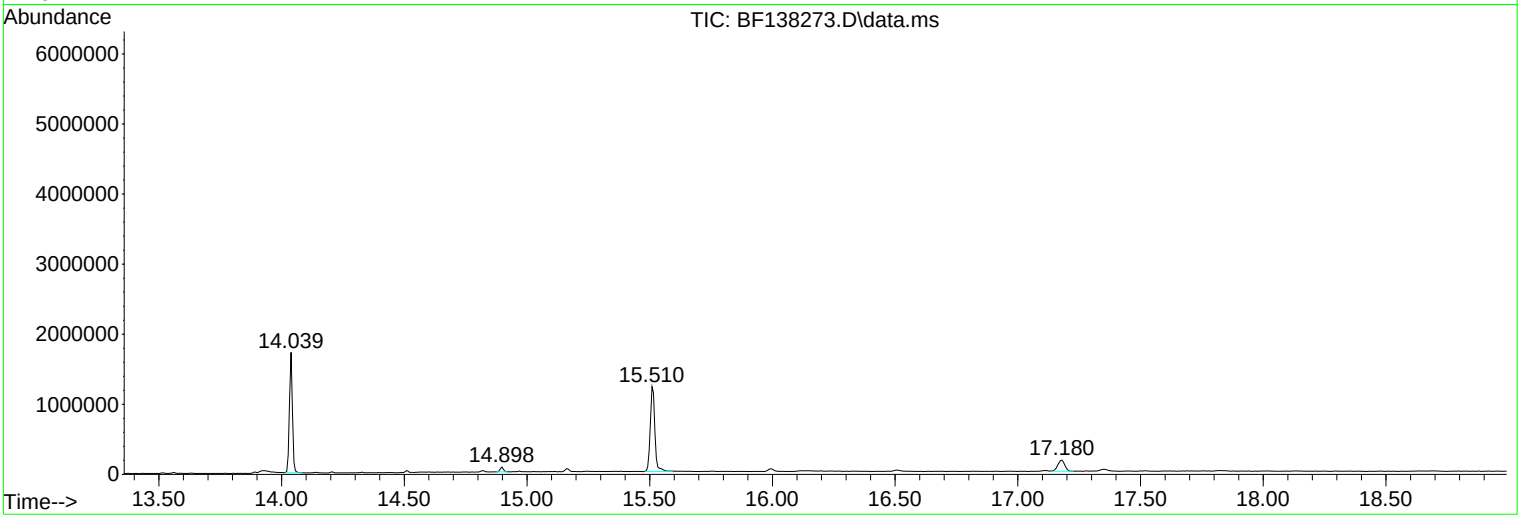
Instrument :
BNA_F
ClientSampleId :
OSTL-C4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.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\BF062024\
Data File : BF138273.D
Acq On : 20 Jun 2024 20:43
Operator : CG\JU
Sample : P2977-16
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OSTL-C4

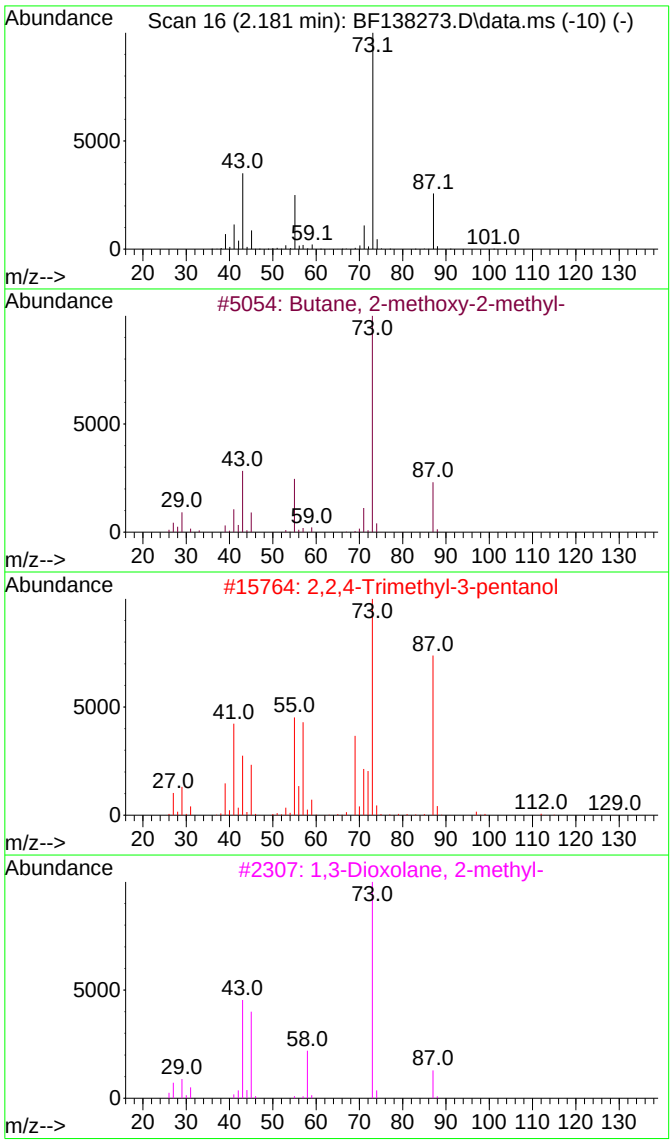
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

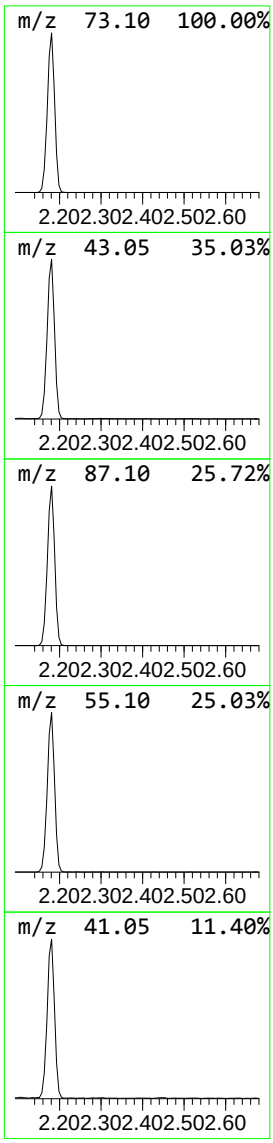
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.181	36.60 ng	2937560	1,4-Dichlorobenzene-d4	6.881

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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062024\
Data File : BF138273.D
Acq On : 20 Jun 2024 20:43
Operator : CG\JU
Sample : P2977-16
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OSTL-C4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

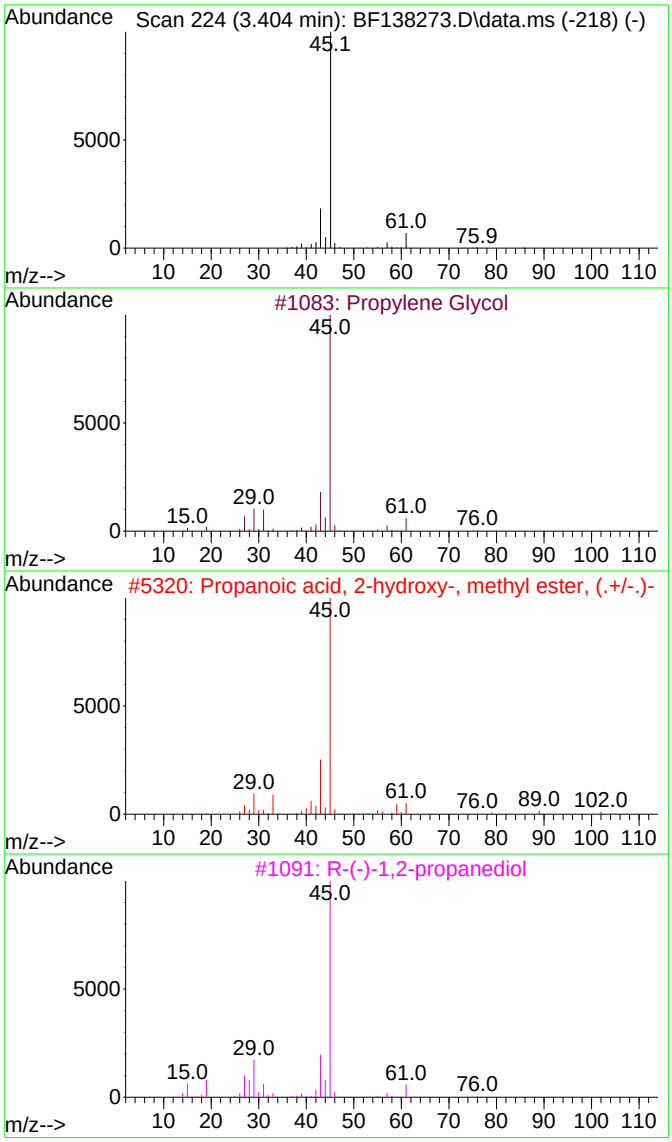
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

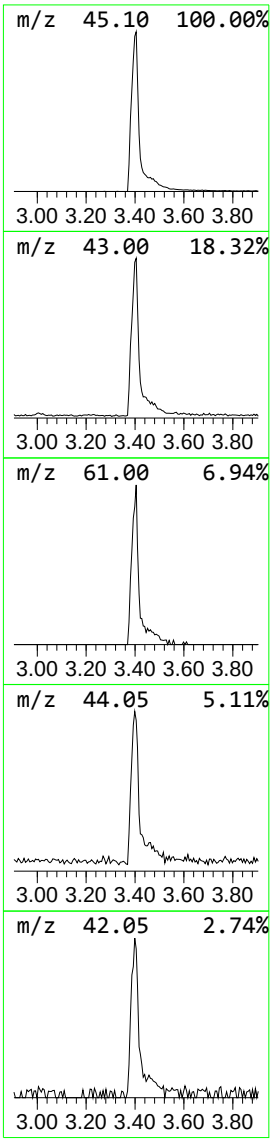
****

Peak Number 2 Propylene Glycol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.404	5.47 ng	438857	1,4-Dichlorobenzene-d4	6.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	90
2	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
3	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062024\
Data File : BF138273.D
Acq On : 20 Jun 2024 20:43
Operator : CG\JU
Sample : P2977-16
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OSTL-C4

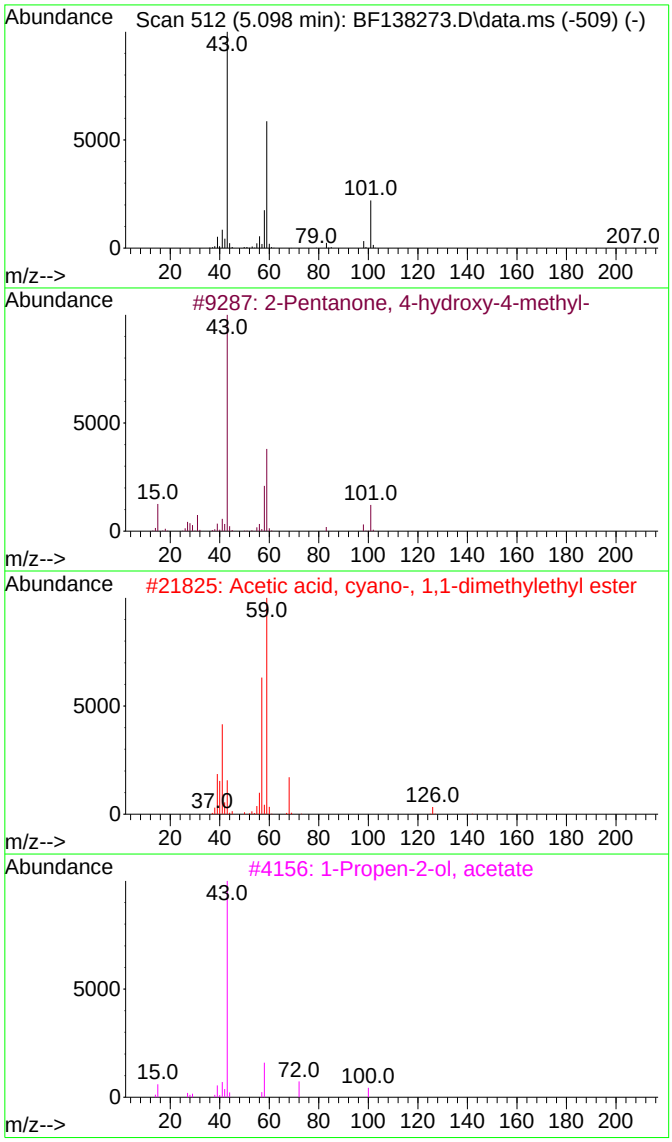
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

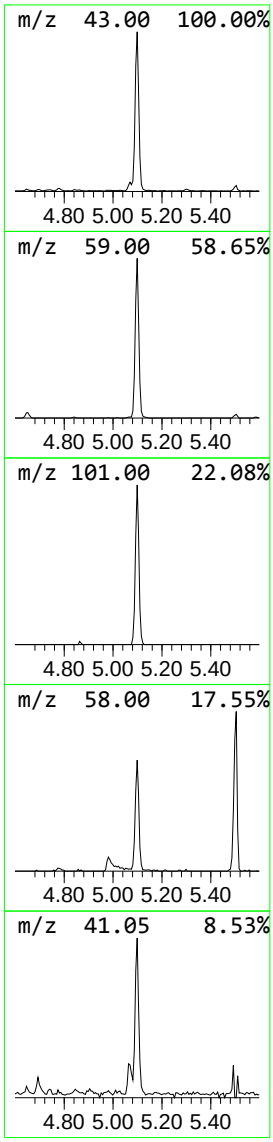
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.098	3.26 ng	261343	1,4-Dichlorobenzene-d4	6.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062024\
Data File : BF138273.D
Acq On : 20 Jun 2024 20:43
Operator : CG\JU
Sample : P2977-16
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OSTL-C4

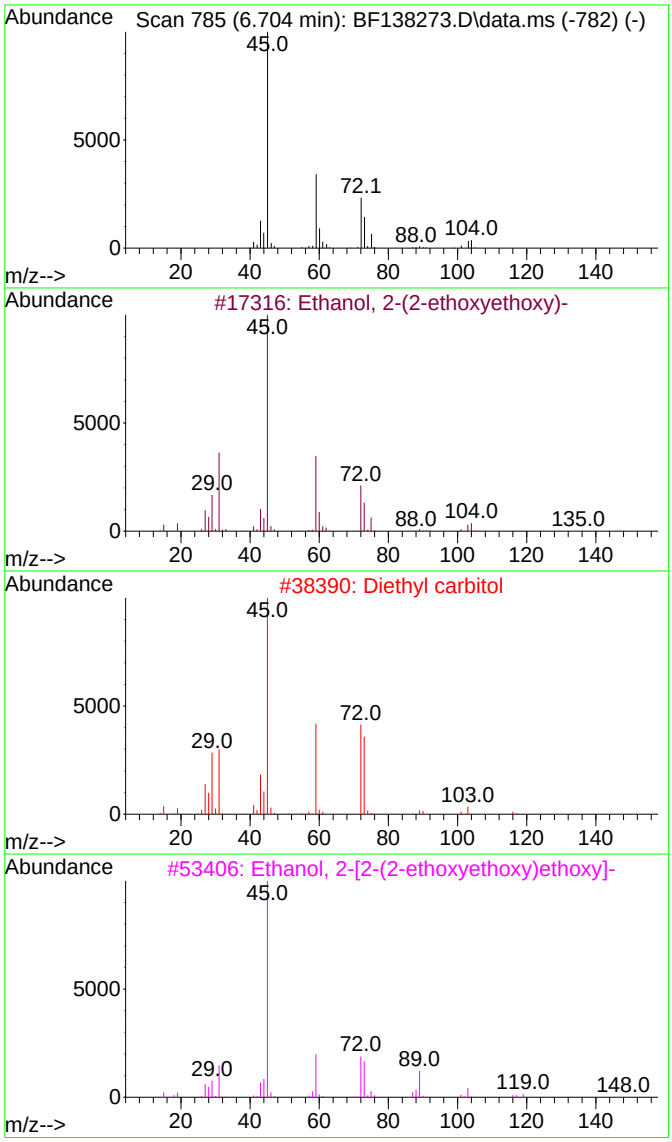
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

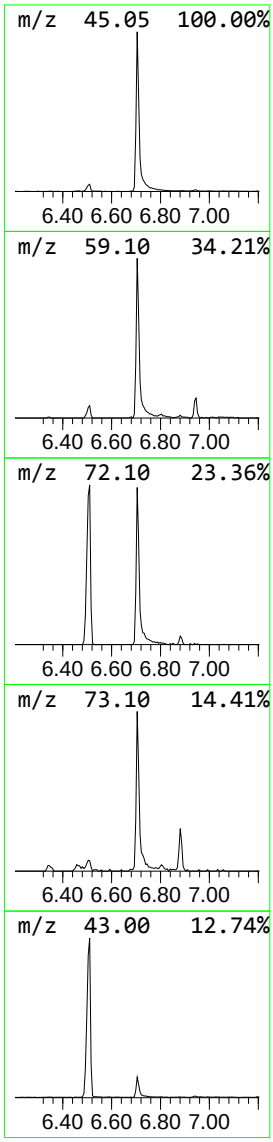
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.704	3.56 ng	286112	1,4-Dichlorobenzene-d4	6.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	90
2	Diethyl carbitol	162	C8H18O3	000112-36-7	72
3	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	50
4	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45
5	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062024\
Data File : BF138273.D
Acq On : 20 Jun 2024 20:43
Operator : CG\JU
Sample : P2977-16
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OSTL-C4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

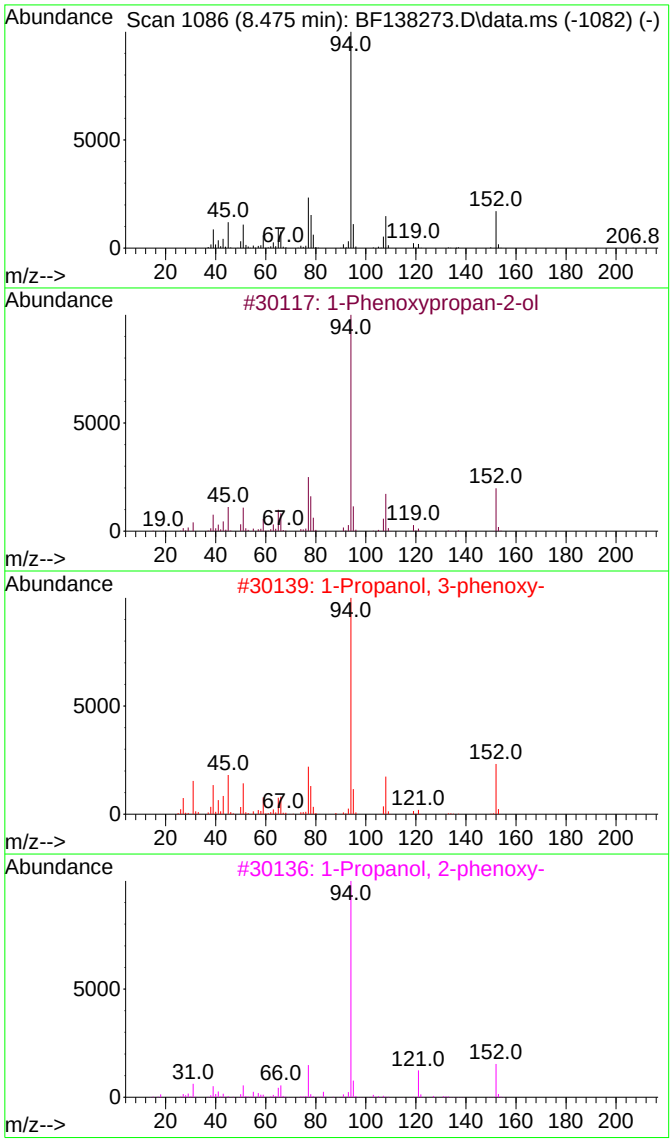
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

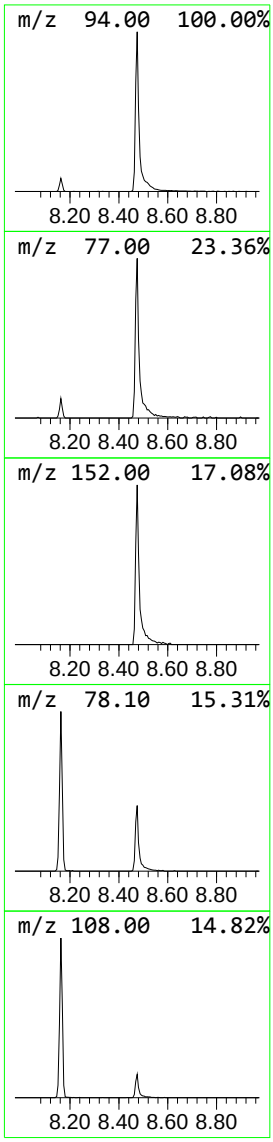
****

Peak Number 5 1-Phenoxypropan-2-ol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.475	4.17 ng	448367	Naphthalene-d8	8.163

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	90
3	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
4	Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	64
5	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062024\
Data File : BF138273.D
Acq On : 20 Jun 2024 20:43
Operator : CG\JU
Sample : P2977-16
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OSTL-C4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

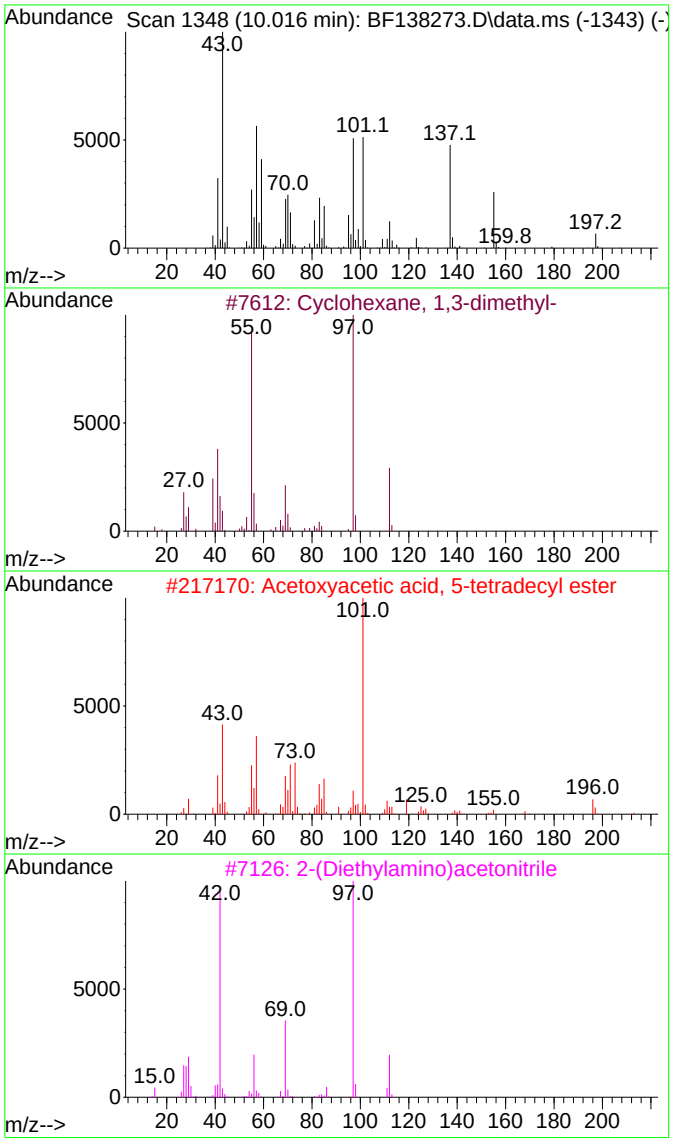
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

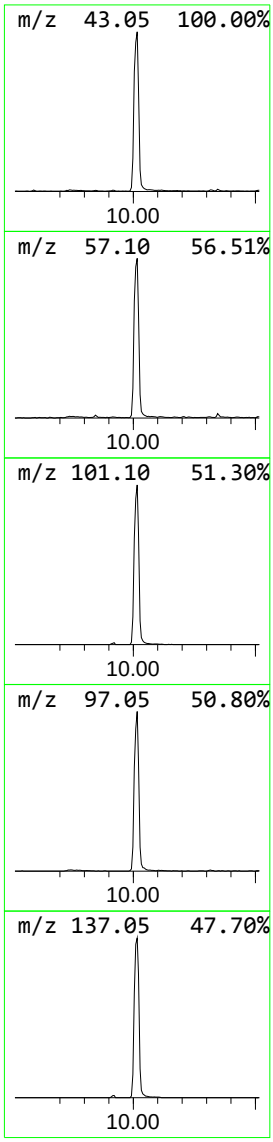
****

Peak Number 6 unknown10.016 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.016	13.03 ng	1622550	Acenaphthene-d10	9.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,3-dimethyl-	112	C8H16	000591-21-9	11
2	Acetoxyacetic acid, 5-tetradecyl...	314	C18H34O4	1000308-81-0	10
3	2-(Diethylamino)acetonitrile	112	C6H12N2	003010-02-4	10
4	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	10
5	7-Oxabicyclo[4.1.0]heptane, 1-me...	112	C7H12O	001713-33-3	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062024\
Data File : BF138273.D
Acq On : 20 Jun 2024 20:43
Operator : CG\JU
Sample : P2977-16
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OSTL-C4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

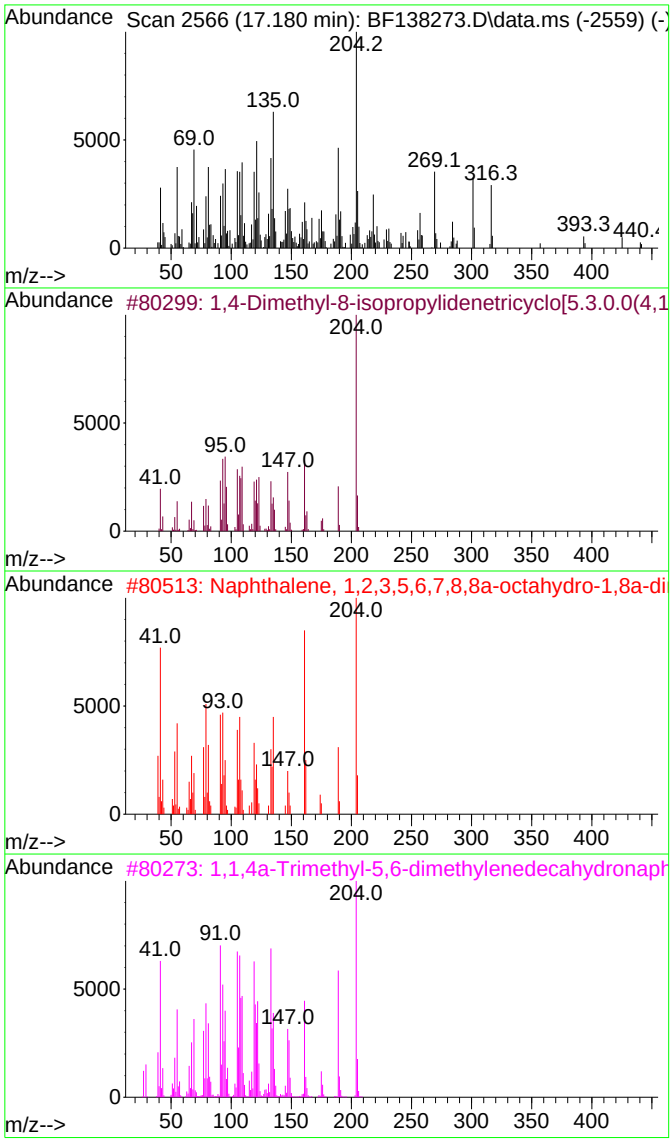
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

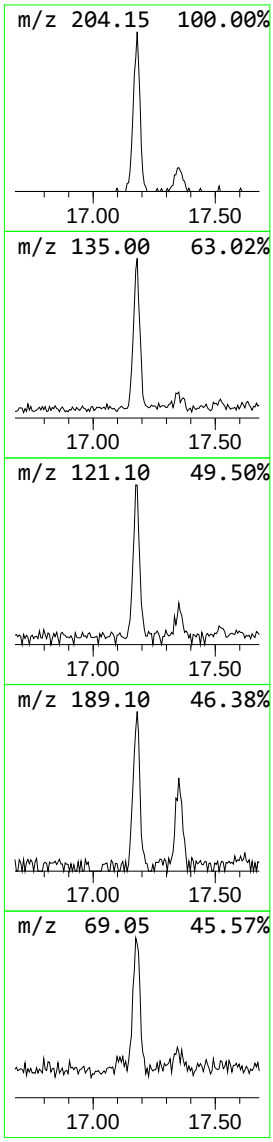
****

Peak Number 7 1,4-Dimethyl-8-isopropylide... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.180	3.96 ng	311495	Perylene-d12	15.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1010140-07-7	70
2	Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	64
3	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	64
4	1H-3a,7-Methanoazulene, octahydr...	204	C15H24	000508-55-4	55
5	1,2,4,8-Tetramethylbicyclo[6.3.0...	204	C15H24	137235-51-9	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062024\
Data File : BF138273.D
Acq On : 20 Jun 2024 20:43
Operator : CG\JU
Sample : P2977-16
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OSTL-C4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.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...	2.181	36.6	ng	2937560	1	6.881	1605350	20.0
Propylene Glycol	3.404	5.5	ng	438857	1	6.881	1605350	20.0
2-Pentanone, 4-...	5.098	3.3	ng	261343	1	6.881	1605350	20.0
Ethanol, 2-(2-e...	6.704	3.6	ng	286112	1	6.881	1605350	20.0
1-Phenoxypropan...	8.475	4.2	ng	448367	2	8.163	2149300	20.0
unknown10.016	10.016	13.0	ng	1622550	3	9.916	2490730	20.0
1,4-Dimethyl-8-...	17.180	4.0	ng	311495	6	15.509	1571510	20.0