LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062624\
Data File : BF138358.D
Acq On : 26 Jun 2024 18:29
Operator : CG\JU
Sample : P2915-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-SOUTH-1

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: BF138358.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	11	19	24	rVB	2848692	3713681	58.99%	8.472%
2	2.305	32	37	41	rBV	49082	63901	1.02%	0.146%
3	3.416	222	226	236	rBV	75861	153590	2.44%	0.350%
4	5.110	510	514	522	rVB	294908	391817	6.22%	0.894%
5	5.510	576	582	585	rBV	4817441	4887487	77.63%	11.150%
6	6.510	746	752	755	rBV	4070322	5077815	80.66%	11.584%
7	6.881	811	815	818	rBV	1419798	1169805	18.58%	2.669%
8	7.445	905	911	914	rBV	3157055	3353144	53.26%	7.650%
9	7.692	949	953	957	rVB	164489	125847	2.00%	0.287%
10	8.157	1025	1032	1036	rBV	1780304	1593912	25.32%	3.636%
11	8.469	1076	1085	1093	rBV	156448	169003	2.68%	0.386%
12	9.233	1210	1215	1218	rBV	6361236	6295557	100.00%	14.362%
13	9.910	1326	1330	1334	rBV	2082532	1755154	27.88%	4.004%
14	10.010	1338	1347	1350	rBV	140557	185047	2.94%	0.422%
15	10.704	1460	1465	1468	rBV	4214561	3880454	61.64%	8.853%
16	11.398	1579	1583	1586	rBV	2112764	1700282	27.01%	3.879%
17	11.922	1668	1672	1686	rBV2	492879	521506	8.28%	1.190%
18	12.704	1802	1805	1817	rBV3	80493	117275	1.86%	0.268%
19	12.986	1848	1853	1856	rBV	6267853	5656886	89.86%	12.905%
20	13.874	2001	2004	2012	rBV	187109	297624	4.73%	0.679%
21	14.033	2025	2031	2035	rBV	1383430	1184810	18.82%	2.703%
22	14.886	2172	2176	2180	rBV	327688	310143	4.93%	0.708%
23	15.504	2275	2281	2290	rBV	998673	1229547	19.53%	2.805%

Sum of corrected areas: 43834287

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062624\
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Misc :
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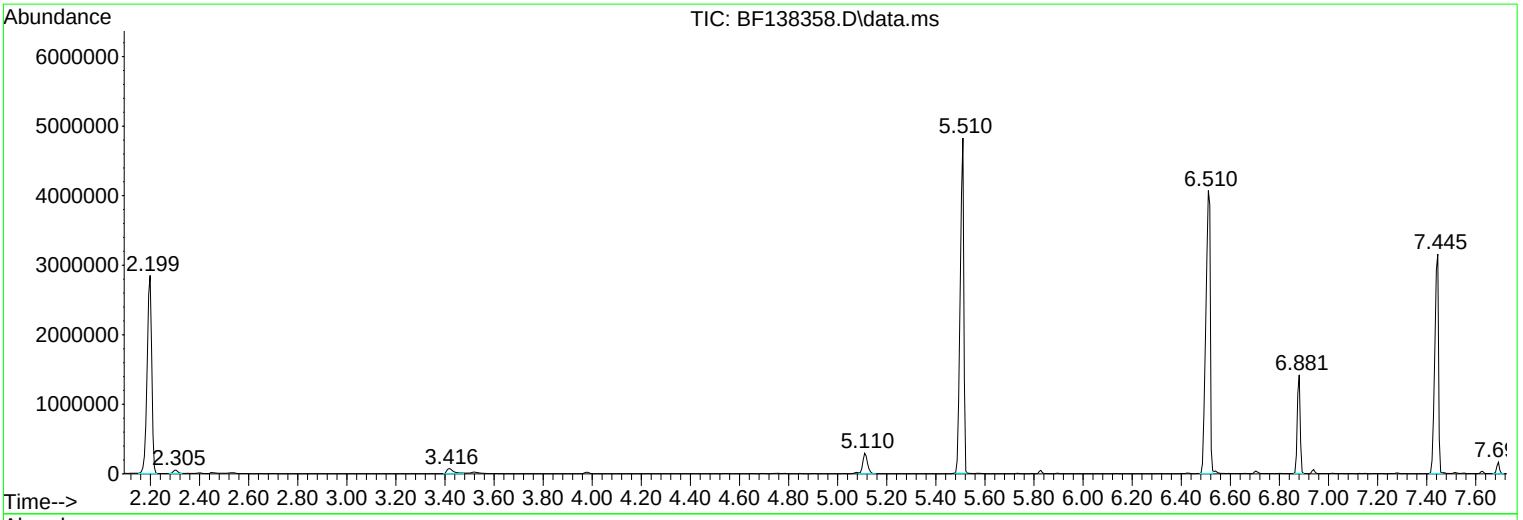
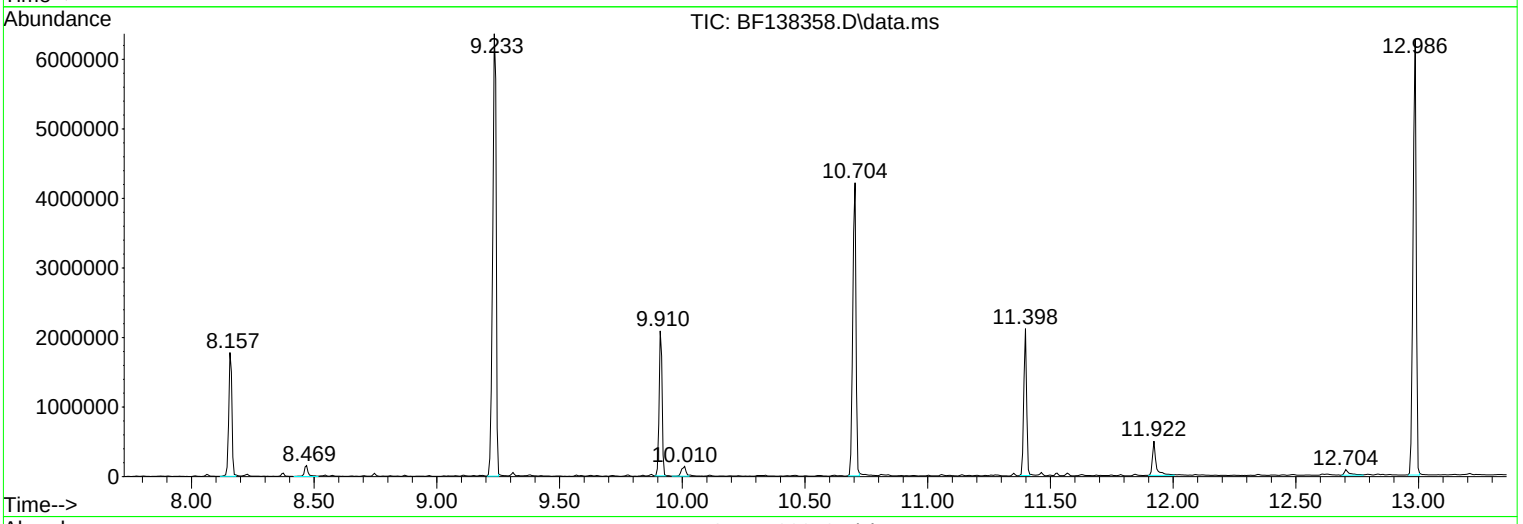
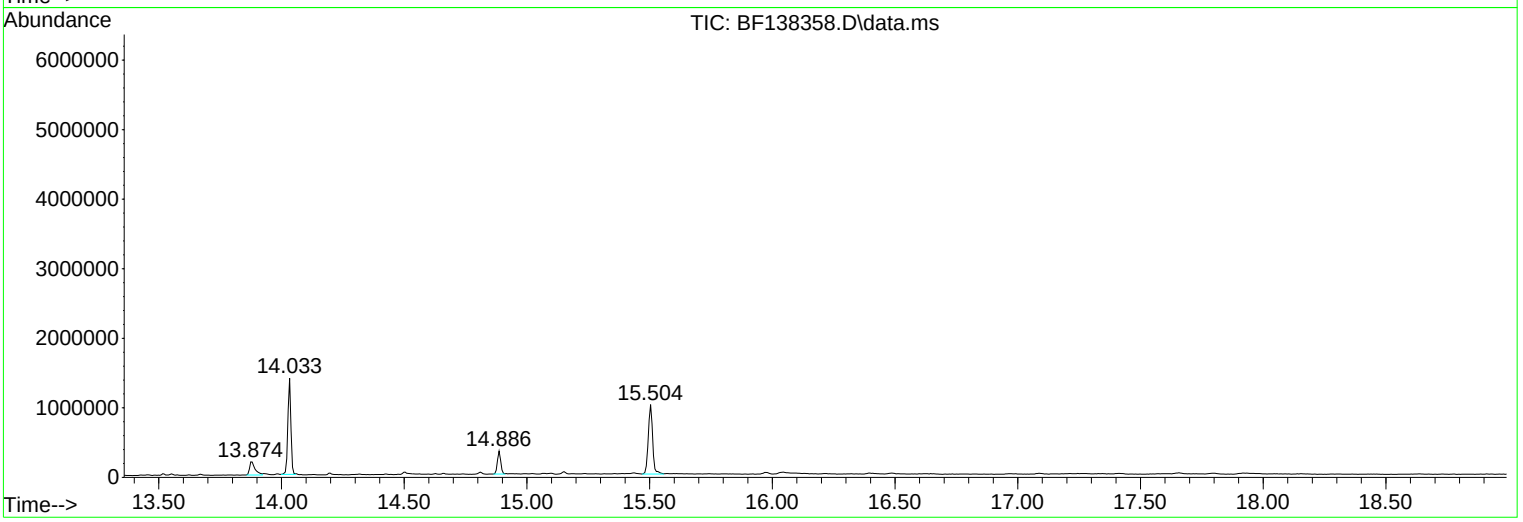
Instrument :
BNA_F
ClientSampleId :
WC-SOUTH-1

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







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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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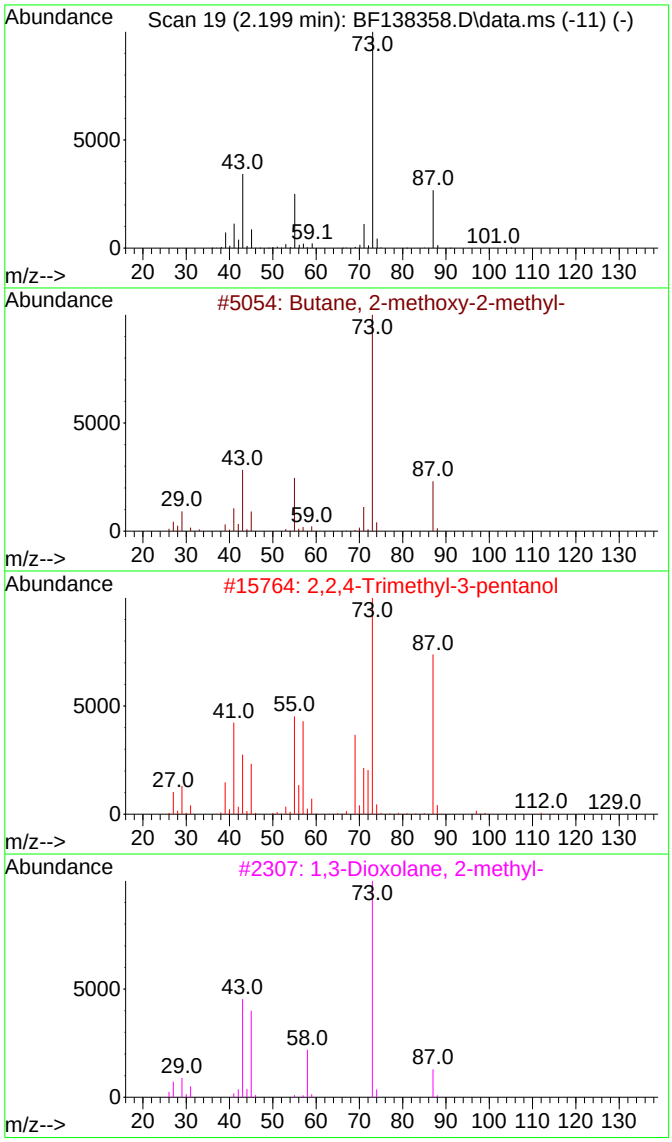
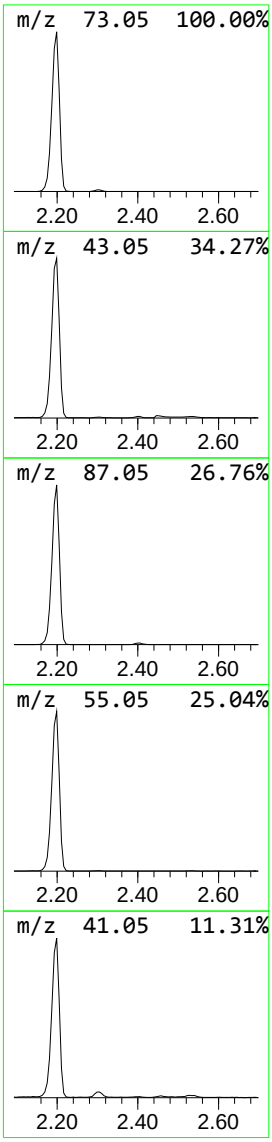
****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.199	63.49 ng	3713680	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





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Data File : BF138358.D
Acq On : 26 Jun 2024 18:29
Operator : CG\JU
Sample : P2915-02
Misc :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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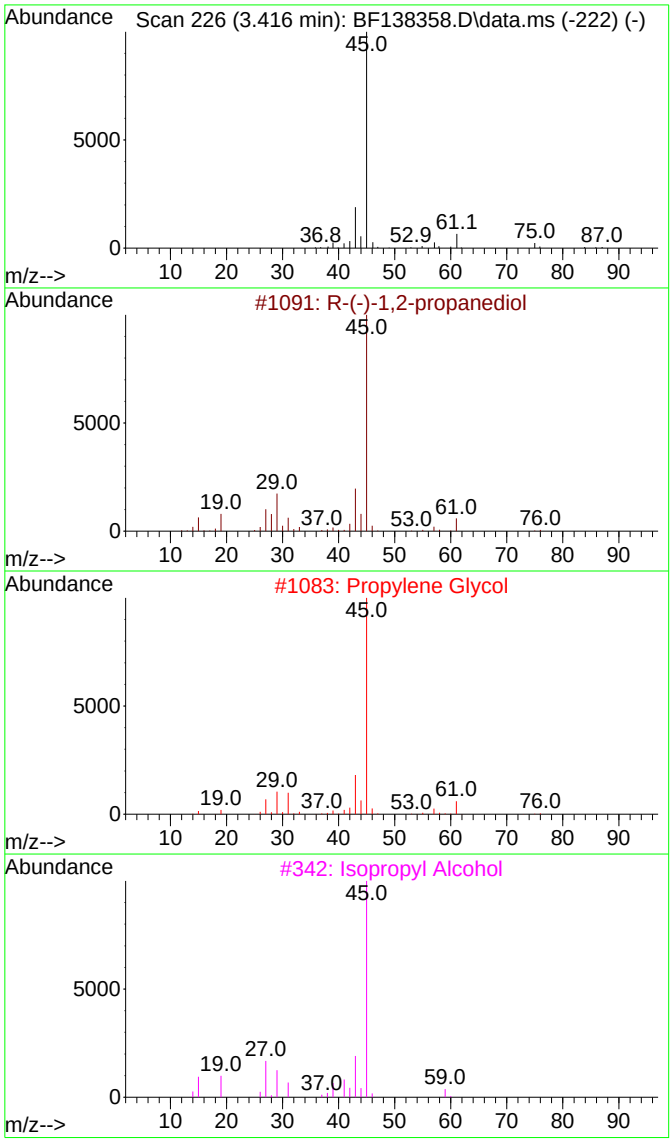
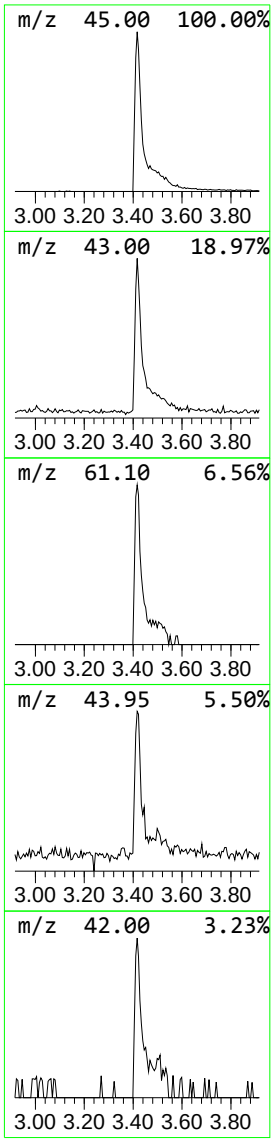
****

Peak Number 2 R-(-)-1,2-propanediol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.416	2.63 ng	153590	1,4-Dichlorobenzene-d4	6.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	80
2	Propylene Glycol	76	C3H8O2	000057-55-6	78
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	50
4	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
5	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40





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Data File : BF138358.D
Acq On : 26 Jun 2024 18:29
Operator : CG\JU
Sample : P2915-02
Misc :
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Instrument :
BNA_F
ClientSampleId :
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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
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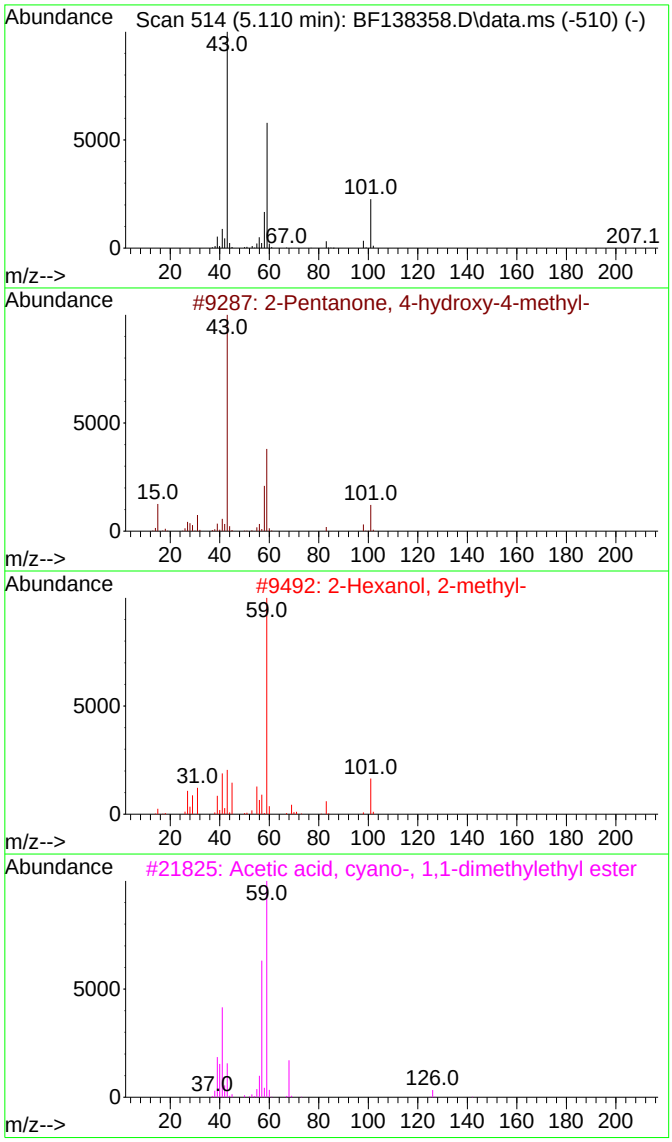
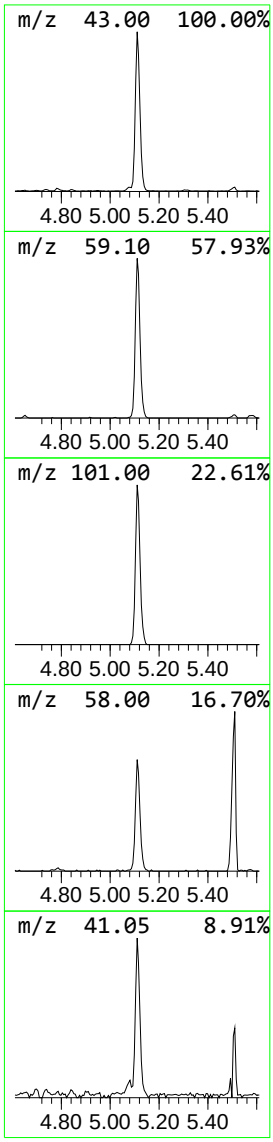
****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	6.70 ng	391817	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	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	23
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





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Data File : BF138358.D
Acq On : 26 Jun 2024 18:29
Operator : CG\JU
Sample : P2915-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-SOUTH-1

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

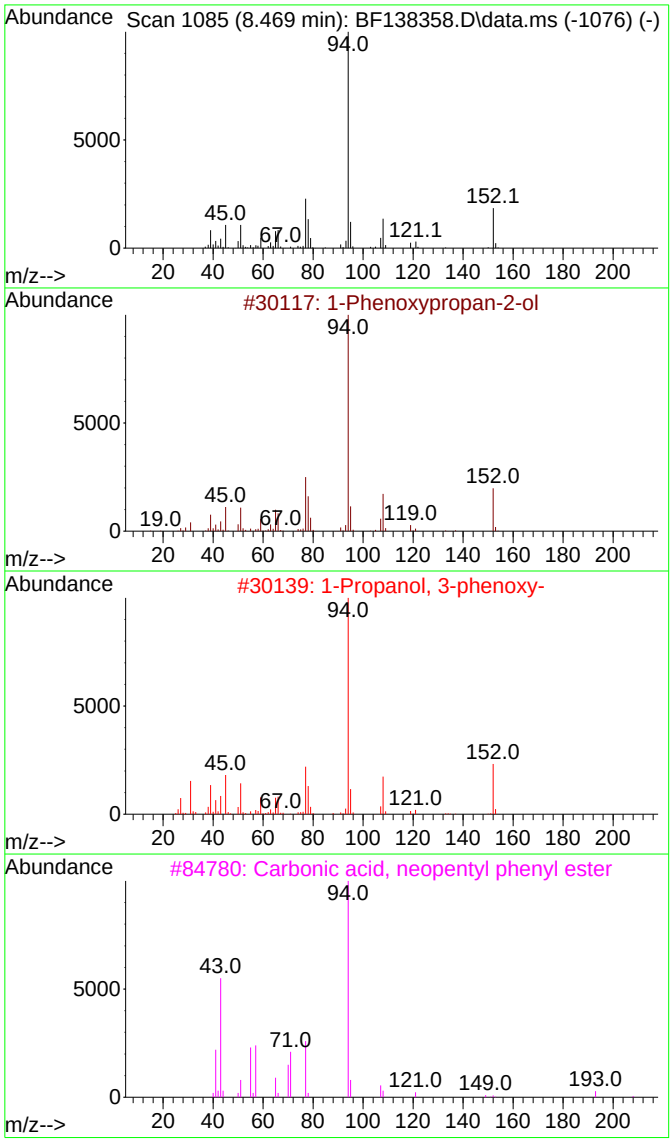
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

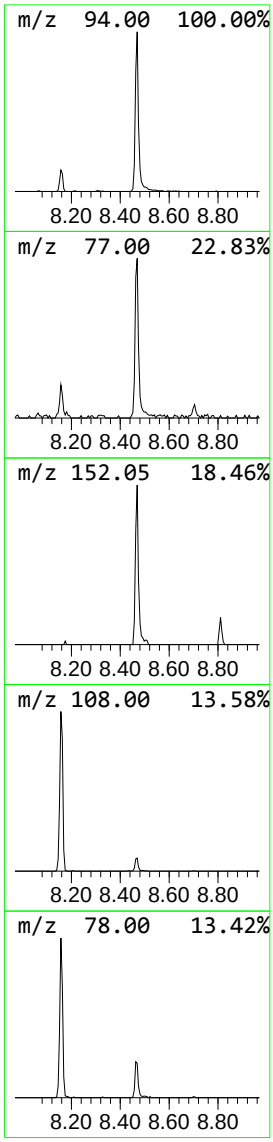
****

Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.469	2.12 ng	169003	Naphthalene-d8	8.157

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





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Operator : CG\JU
Sample : P2915-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-SOUTH-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
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TIC Library : C:\Database\NIST20.L
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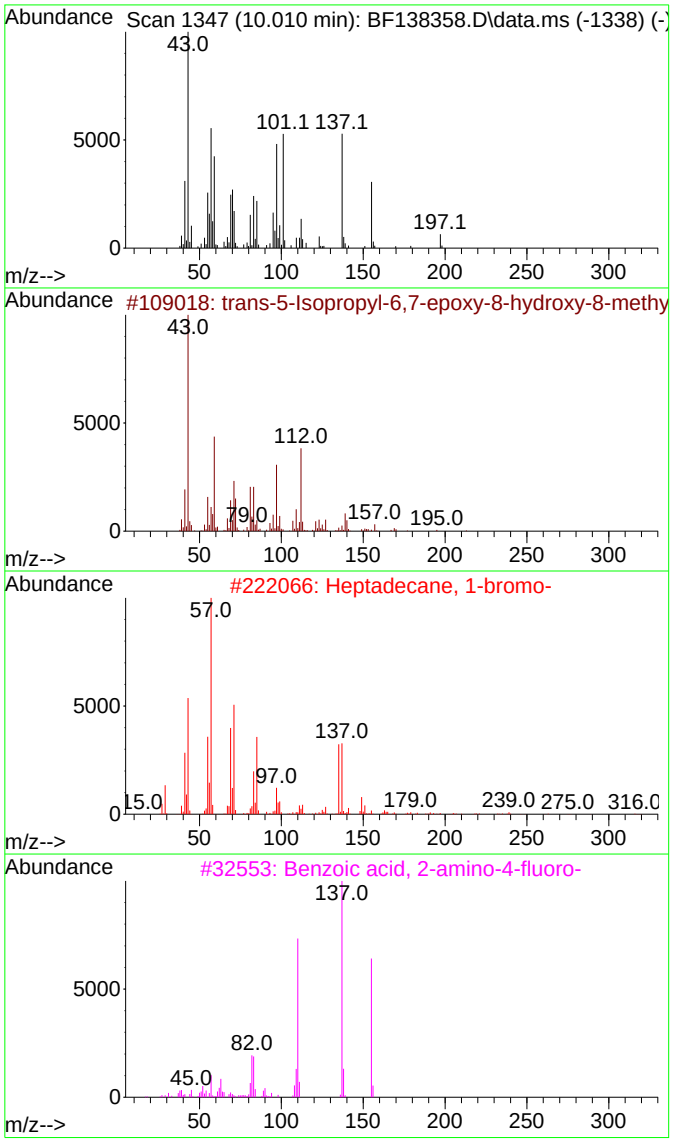
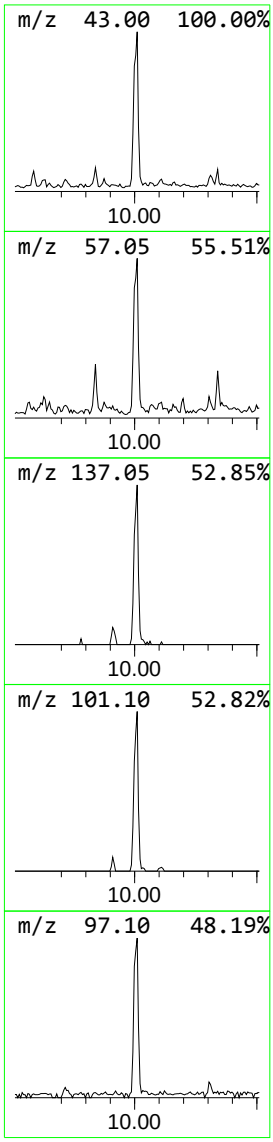
****

Peak Number 5 unknown10.010 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.010	2.11 ng	185047	Acenaphthene-d10	9.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-5-Isopropyl-6,7-epoxy-8-hy...	228	C13H24O3	058002-07-6	12
2	Heptadecane, 1-bromo-	318	C17H35Br	003508-00-7	10
3	Benzoic acid, 2-amino-4-fluoro-	155	C7H6FNO2	000446-32-2	10
4	Amyl tiglate	170	C10H18O2	007785-65-1	10
5	2-Amino-5-fluorobenzoic acid	155	C7H6FNO2	000446-08-2	10





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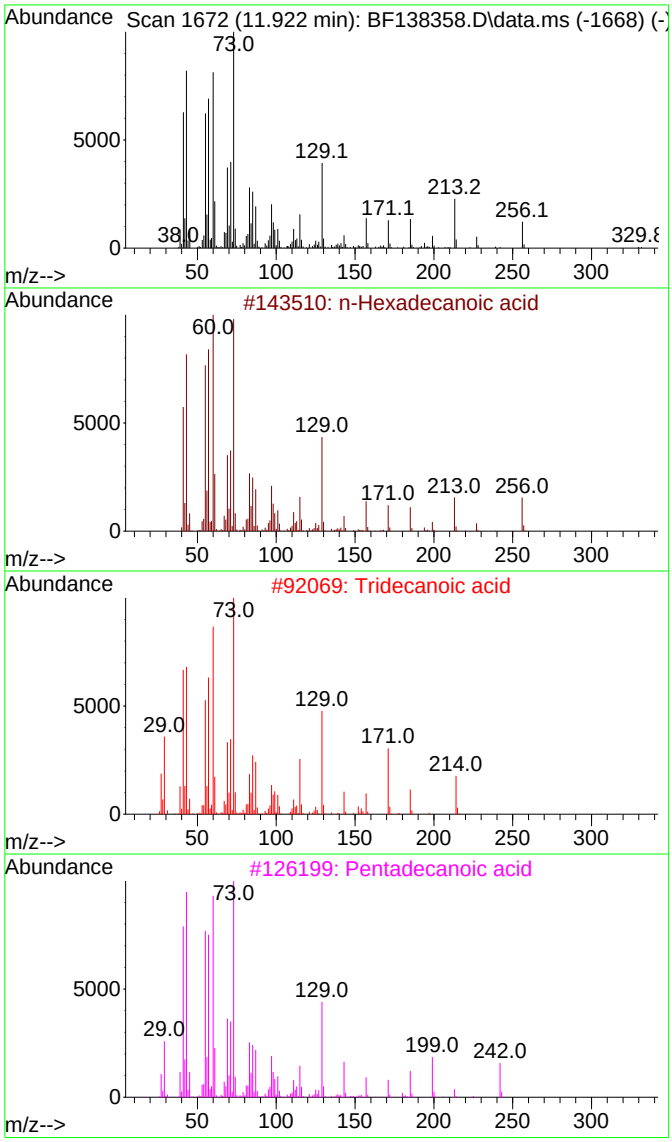
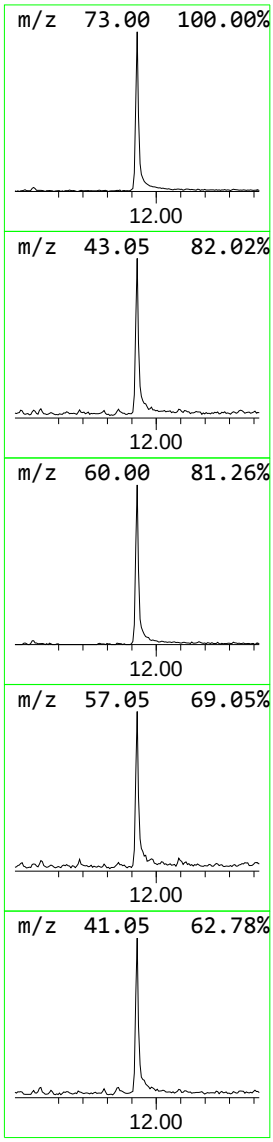
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	6.13 ng	521506	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
5	Octadecanoic acid	284	C18H36O2	000057-11-4	90





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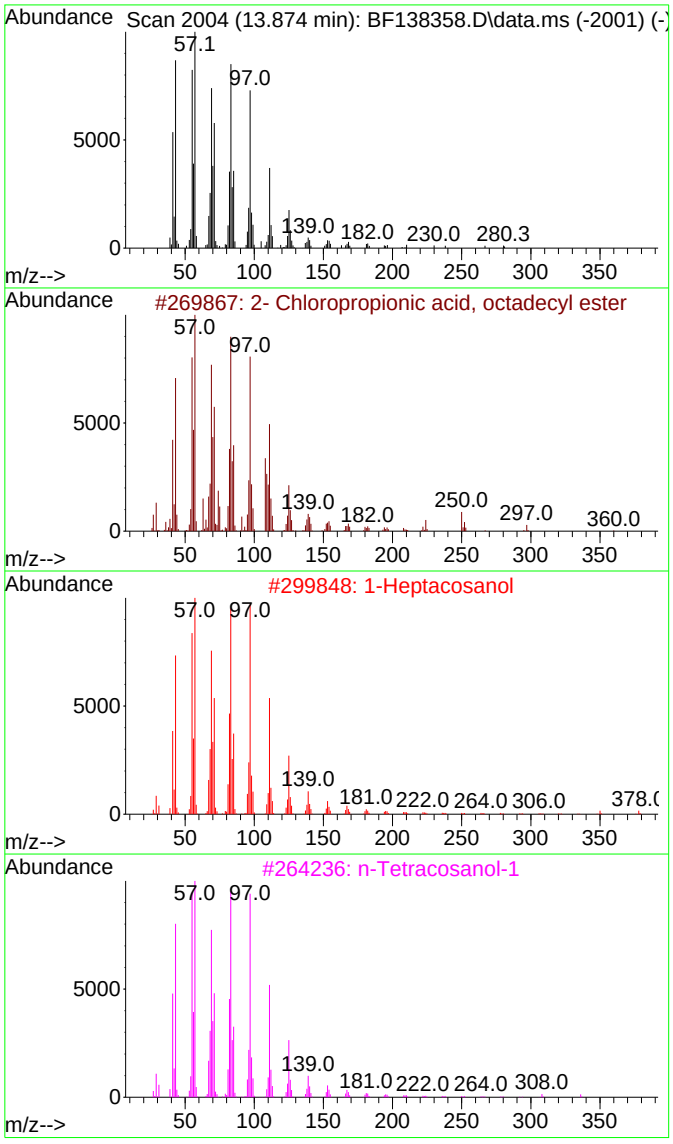
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

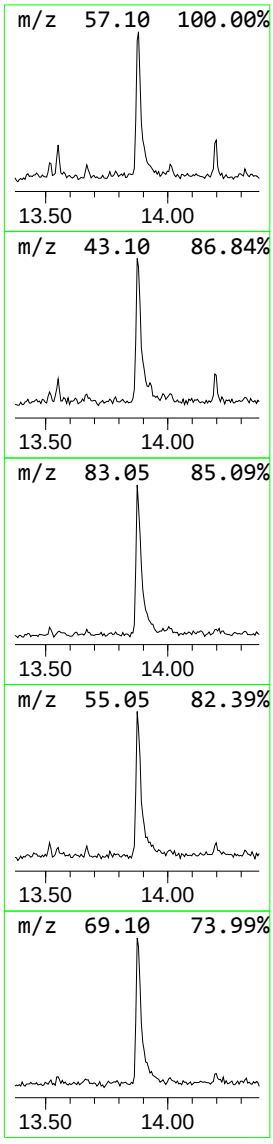
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 2- Chloropropionic acid, oc... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	5.02 ng	297624	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
2	1-Heptacosanol	396	C27H56O	002004-39-9	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	1-Hexacosene	364	C26H52	018835-33-1	94
5	1-Heneicosanol	312	C21H44O	015594-90-8	94





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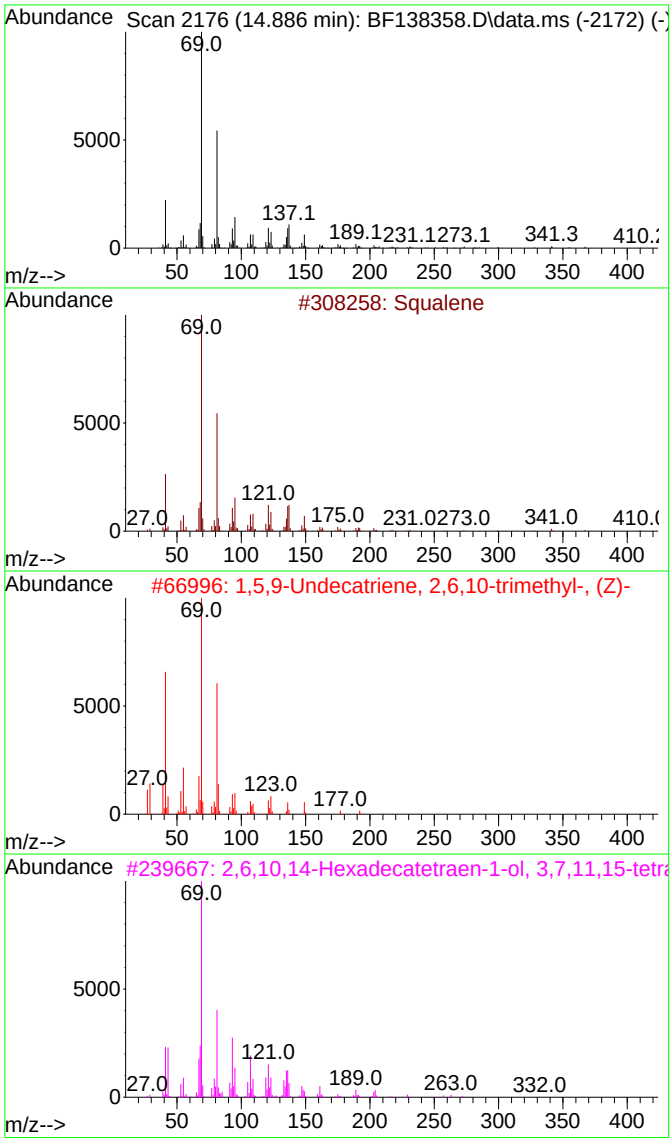
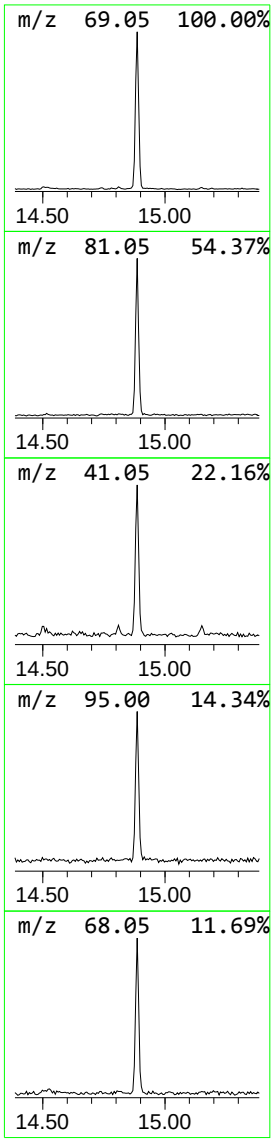
****

Peak Number 8 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.886	5.04 ng	310143	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	96
2	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	87
3	2,6,10,14-Hexadecatetraen-1-ol, ...	332	C22H36O2	061691-98-3	78
4	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64





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...	2.199	63.5	ng	3713680	1	6.881	1169810	20.0
R-(-)-1,2-propa...	3.416	2.6	ng	153590	1	6.881	1169810	20.0
2-Pentanone, 4-...	5.110	6.7	ng	391817	1	6.881	1169810	20.0
1-Phenoxypropan...	8.469	2.1	ng	169003	2	8.157	1593910	20.0
unknown10.010	10.010	2.1	ng	185047	3	9.910	1755150	20.0
n-Hexadecanoic ...	11.922	6.1	ng	521506	4	11.398	1700280	20.0
2- Chloropropio...	13.874	5.0	ng	297624	5	14.033	1184810	20.0
Squalene	14.886	5.0	ng	310143	6	15.504	1229550	20.0