LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081424\
Data File : BF138992.D
Acq On : 14 Aug 2024 14:08
Operator : RC/JU
Sample : P3474-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-B2-COMP

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: BF138992.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	20	rVB	564652	784953	62.89%	9.544%
2	2.234	20	24	30	rVB	9613	14951	1.20%	0.182%
3	3.404	218	223	250	rBV	6399	30703	2.46%	0.373%
4	5.063	500	505	531	rVB	69298	114630	9.18%	1.394%
5	5.469	569	574	598	rBV	839962	1130060	90.54%	13.740%
6	6.481	741	746	768	rBV	875630	1167905	93.57%	14.200%
7	6.834	802	806	813	rVB	182425	223016	17.87%	2.712%
8	7.404	897	903	915	rBV	560387	755472	60.53%	9.186%
9	8.116	1019	1024	1037	rVB	229847	287930	23.07%	3.501%
10	8.433	1073	1078	1091	rBV	27674	46415	3.72%	0.564%
11	9.186	1200	1206	1211	rBV	1023072	1248192	100.00%	15.177%
12	9.869	1317	1322	1327	rBV	246464	316373	25.35%	3.847%
13	9.957	1331	1337	1343	rBV	27948	43383	3.48%	0.527%
14	10.657	1451	1456	1469	rBV	511149	673946	53.99%	8.194%
15	11.357	1570	1575	1585	rVB	209868	274975	22.03%	3.343%
16	11.880	1660	1664	1671	rBV6	8975	16887	1.35%	0.205%
17	12.933	1838	1843	1848	rBV	599034	751194	60.18%	9.134%
18	13.863	1991	2001	2016	rBV8	6291	25933	2.08%	0.315%
19	13.998	2019	2024	2036	rVB	128517	166436	13.33%	2.024%
20	15.462	2266	2273	2283	rBV	91342	151114	12.11%	1.837%

Sum of corrected areas: 8224468

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Misc :
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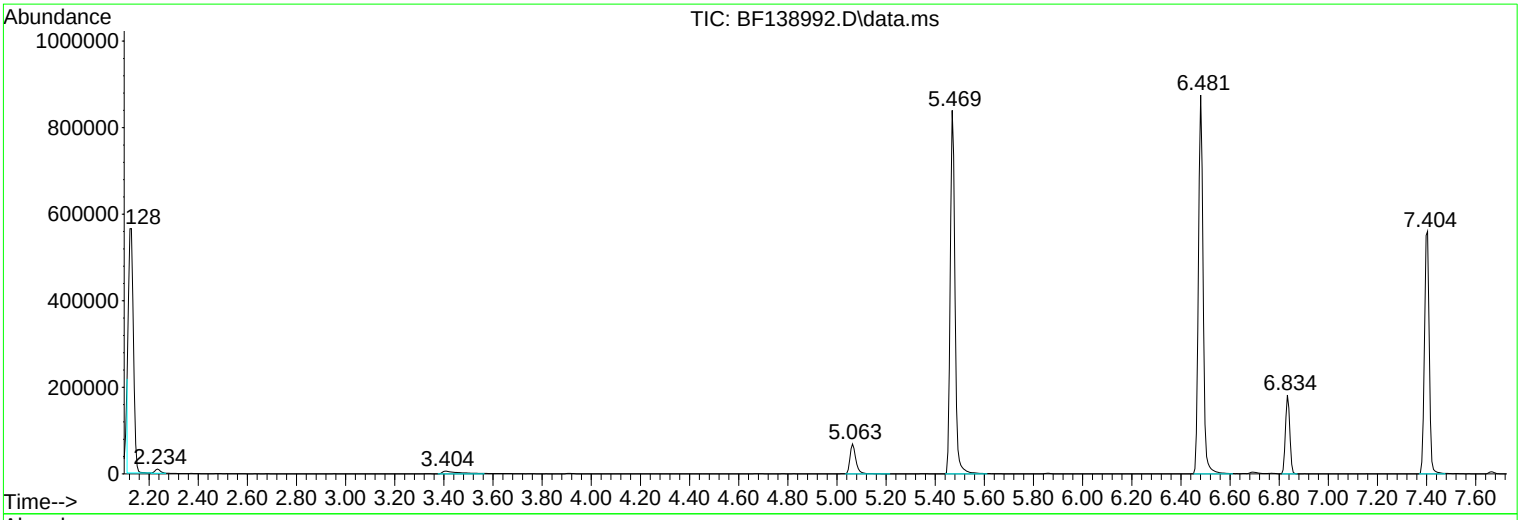
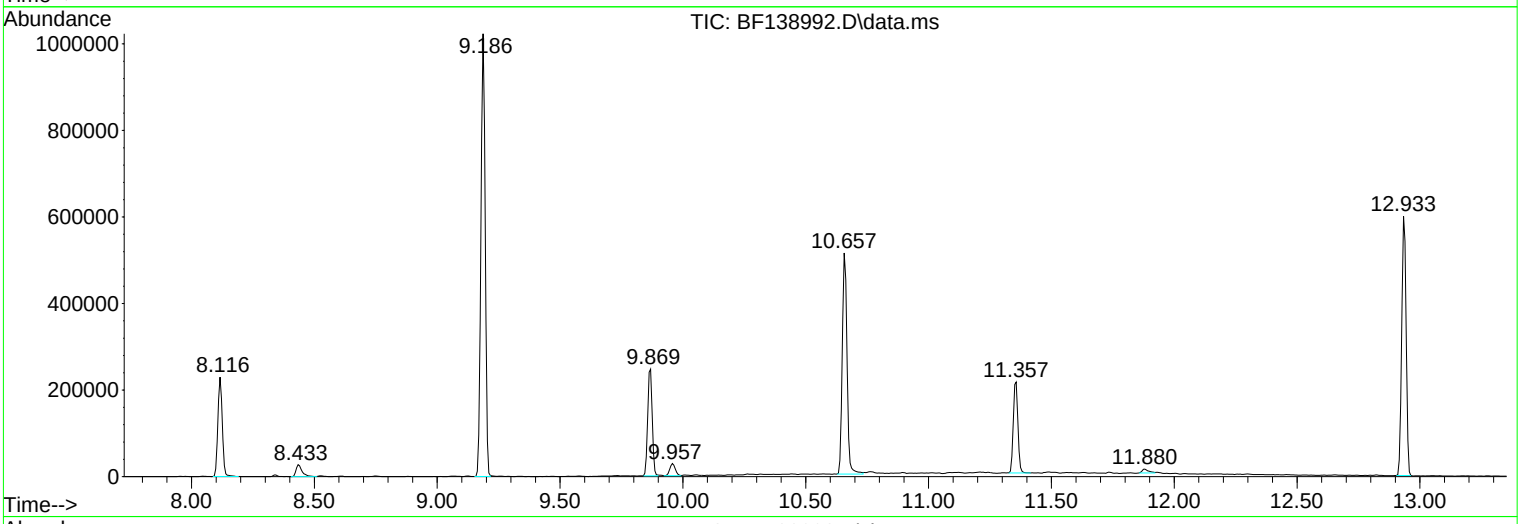
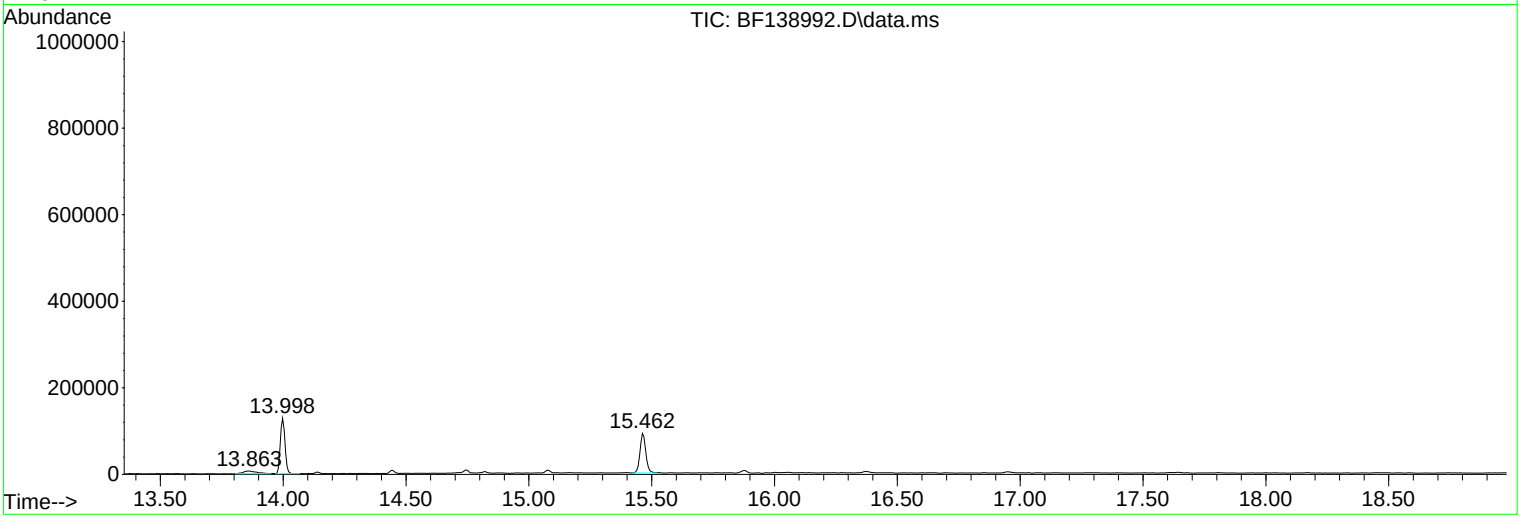
Instrument :
BNA_F
ClientSampleId :
WC-B2-COMP

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

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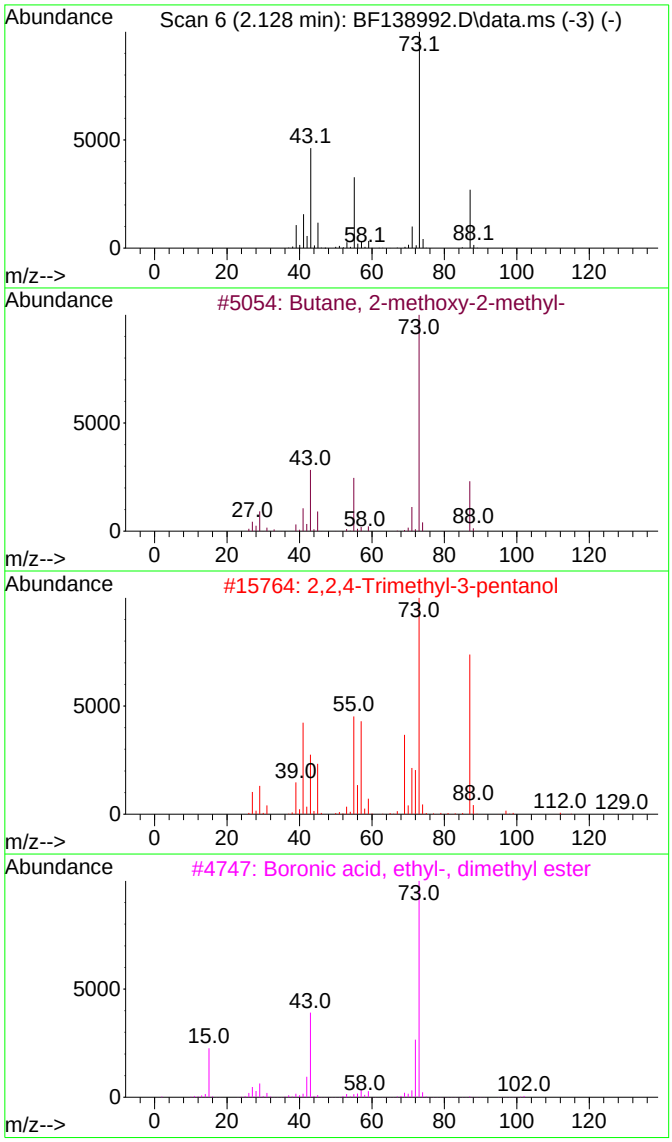
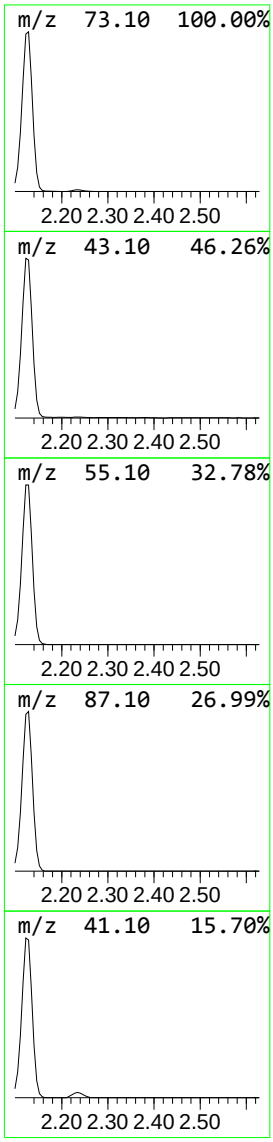
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.128	70.39 ng	784953	1,4-Dichlorobenzene-d4	6.834

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	Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	25
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





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Acq On : 14 Aug 2024 14:08
Operator : RC/JU
Sample : P3474-10
Misc :
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BNA_F
ClientSampleId :
WC-B2-COMP

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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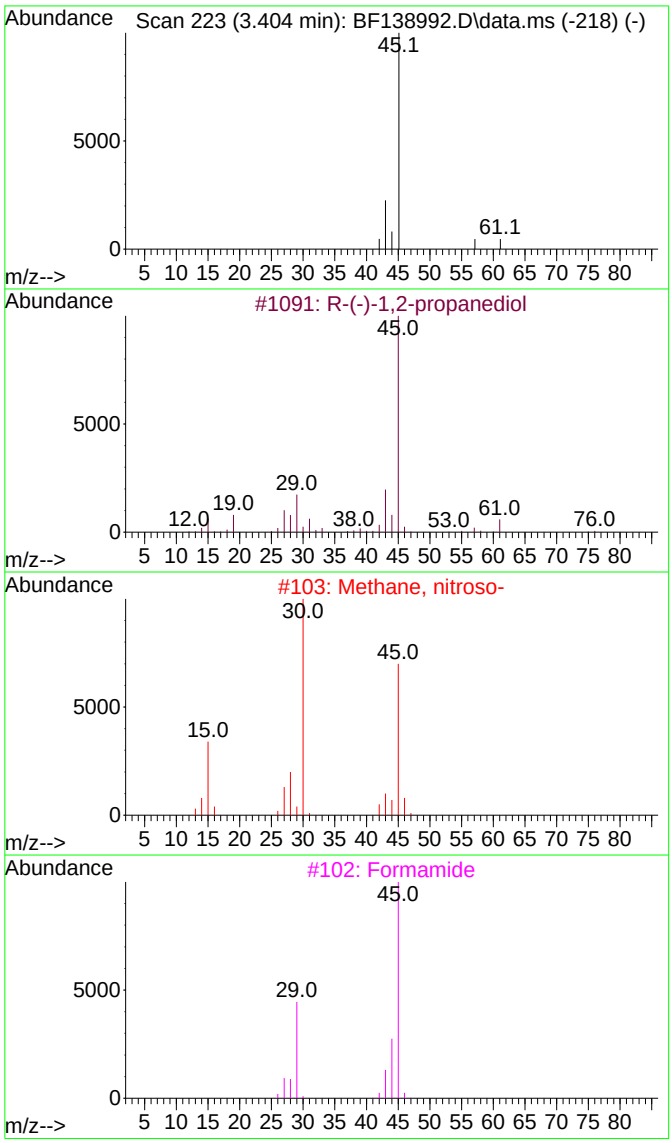
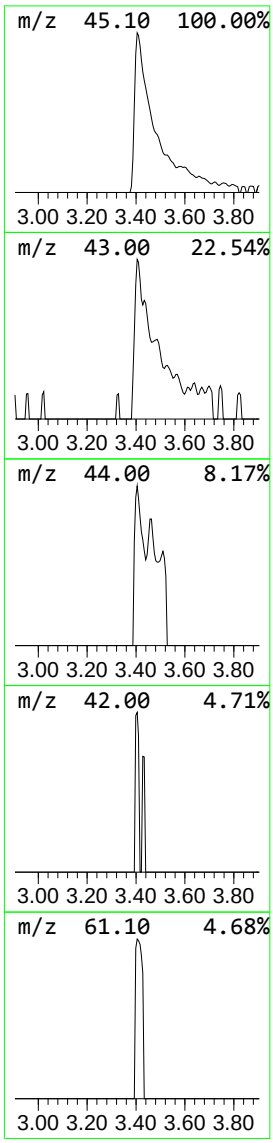
****

Peak Number 2 unknown3.404 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.404	2.75 ng	30703	1,4-Dichlorobenzene-d4	6.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	4
2	Methane, nitroso-	45	CH3NO	000865-40-7	3
3	Formamide	45	CH3NO	000075-12-7	3
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	2
5	Propylene Glycol	76	C3H8O2	000057-55-6	2





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Operator : RC/JU
Sample : P3474-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-B2-COMP

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

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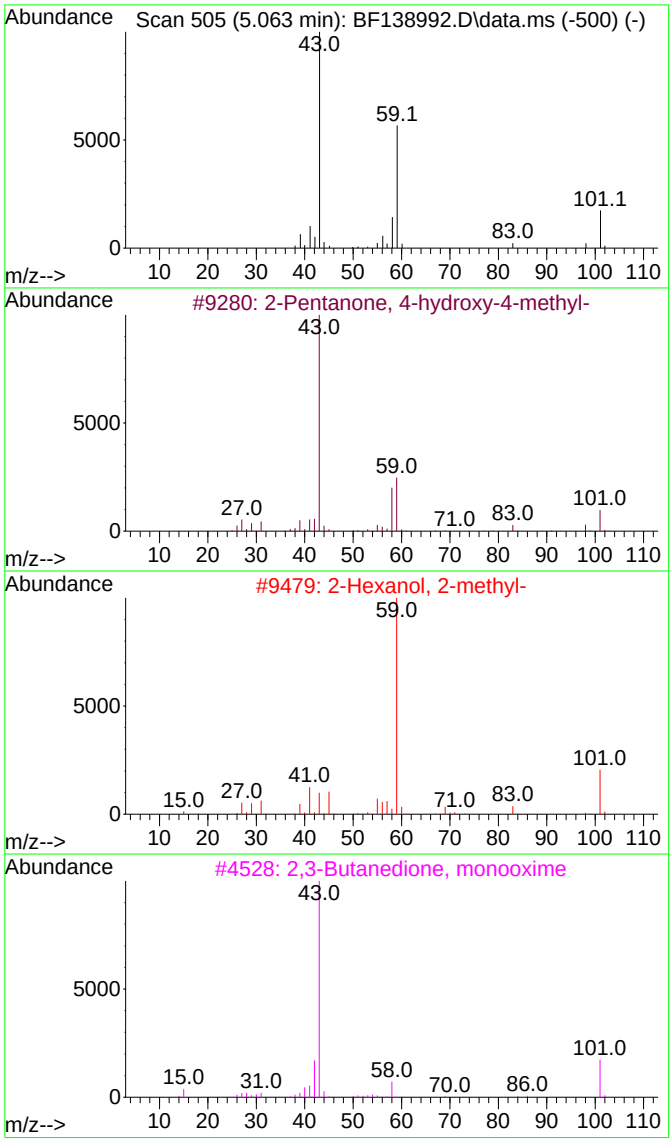
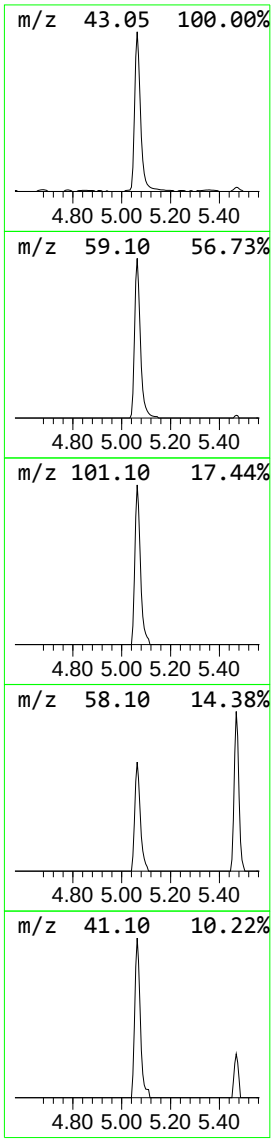
****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.063	10.28 ng	114630	1,4-Dichlorobenzene-d4	6.834

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	28
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Sample : P3474-10
Misc :
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Instrument :
BNA_F
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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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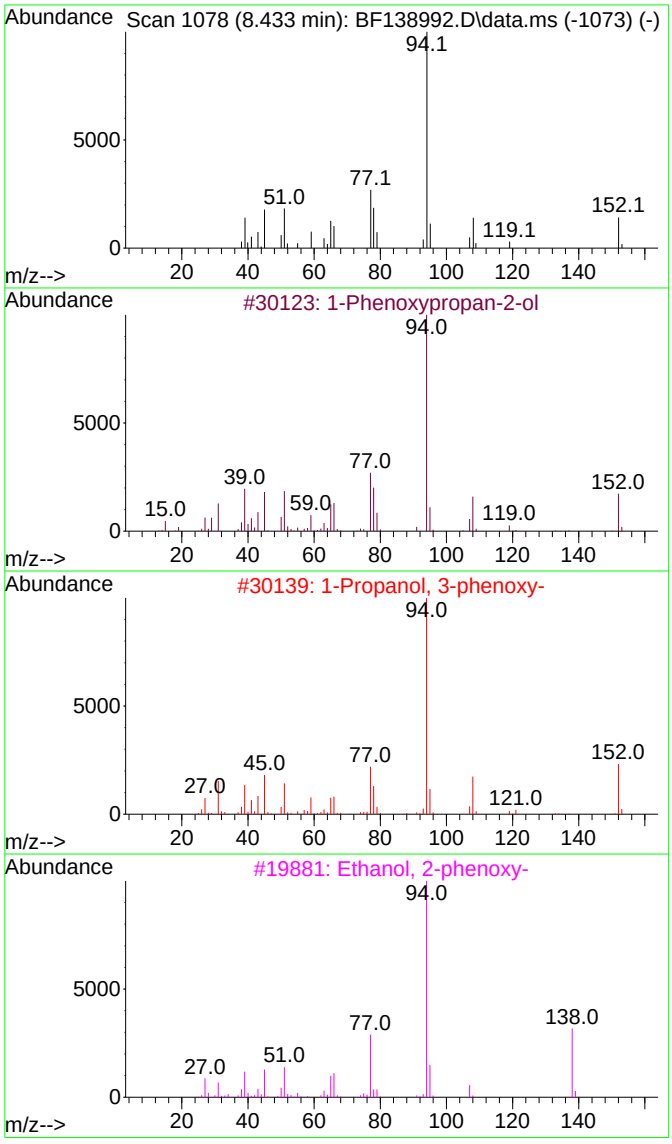
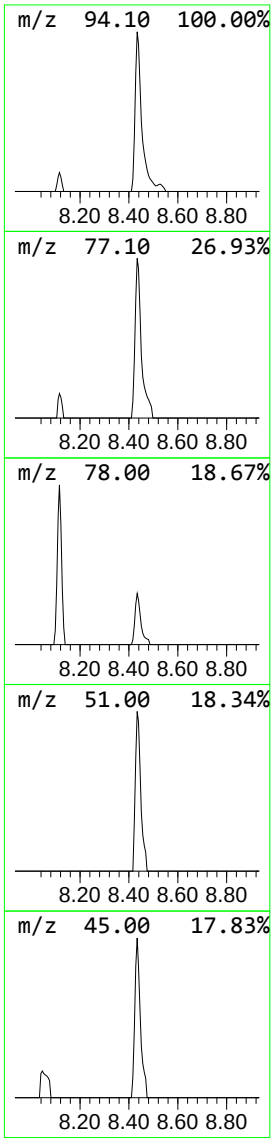
Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.433	3.22 ng	46415	Naphthalene-d8	8.116

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	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59
5	Benzene, (2-methylpropoxy)-	150	C10H14O	001126-75-6	53





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Instrument :
BNA_F
ClientSampleId :
WC-B2-COMP

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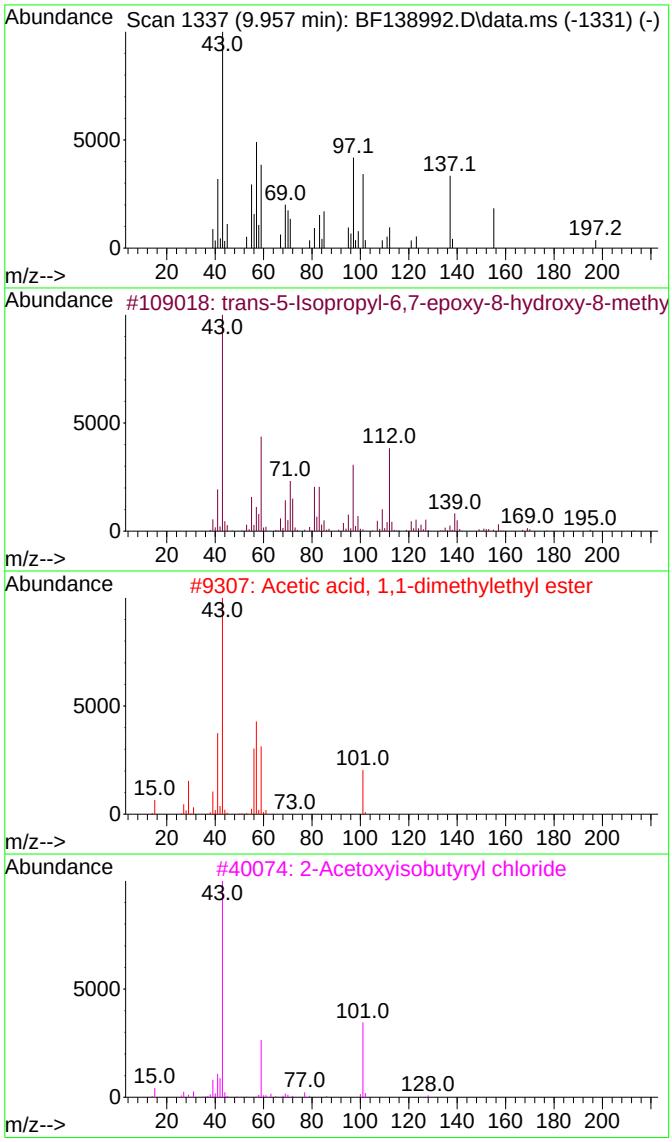
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

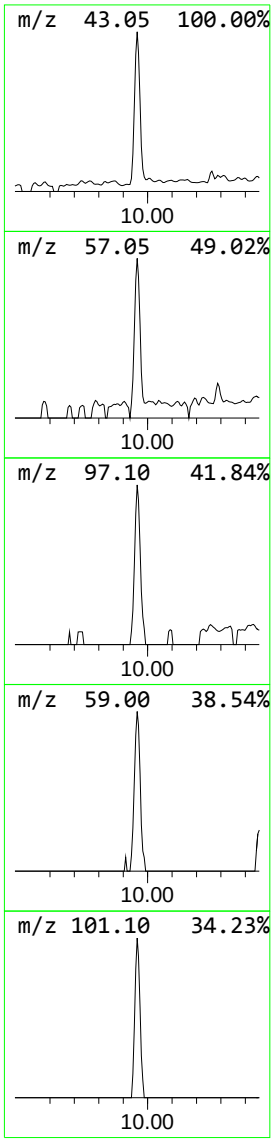
****

Peak Number 5 unknown9.957 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.957	2.74 ng	43383	Acenaphthene-d10	9.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-5-Isopropyl-6,7-epoxy-8-hy...	228	C13H24O3	058002-07-6	17
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	12
3	2-Acetoxyisobutyryl chloride	164	C6H9ClO3	040635-66-3	12
4	17-Pentatriacontene	491	C35H70	006971-40-0	12
5	Hexanoic acid, 3-oxo-, methyl ester	144	C7H12O3	030414-54-1	10





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BNA_F
ClientSampleId :
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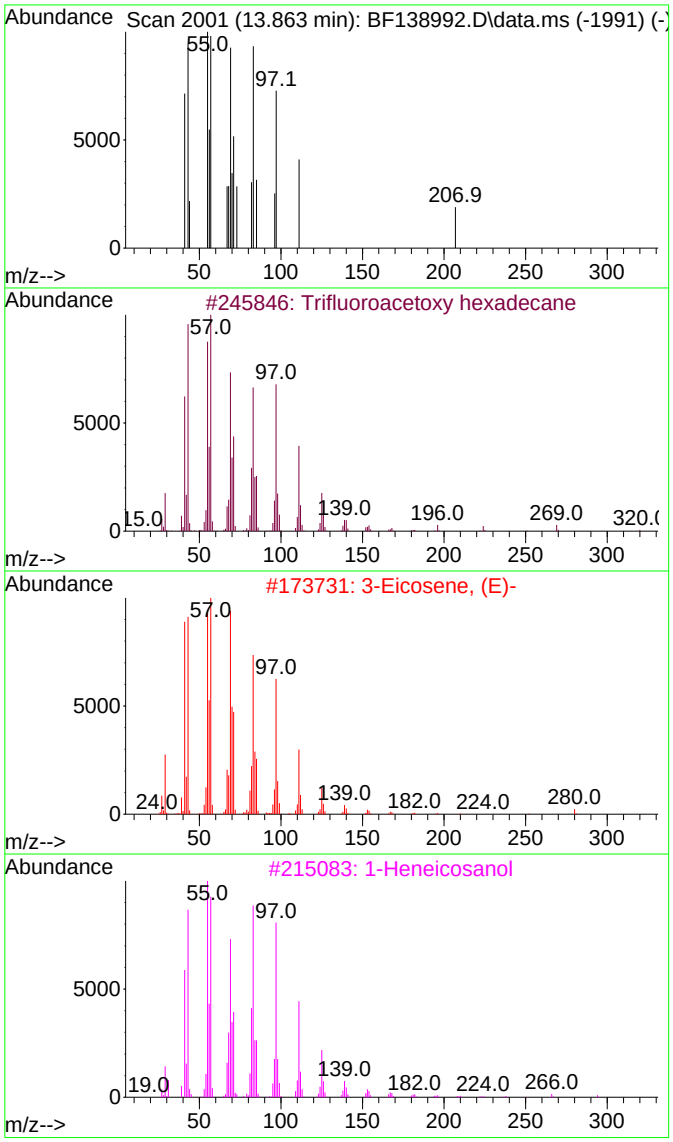
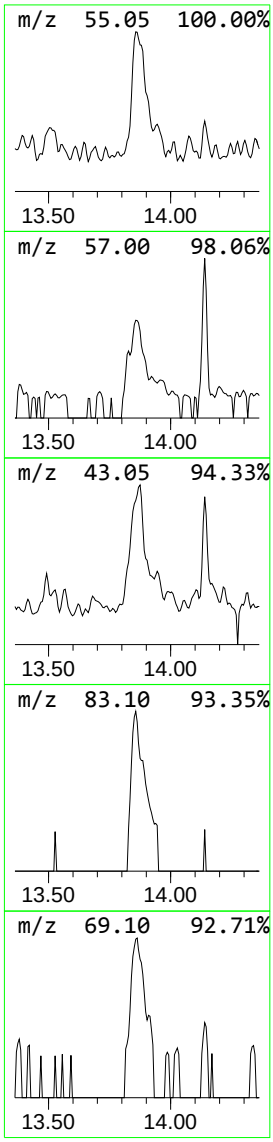
****

Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.863	3.12 ng	25933	Chrysene-d12	13.998

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	87
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	87
3	1-Heneicosanol	312	C21H44O	015594-90-8	87
4	1-Tricosene	322	C23H46	018835-32-0	87
5	1-Heptadecene	238	C17H34	006765-39-5	86





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	70.4	ng	784953	1	6.834	223016	20.0
unknown3.404	3.404	2.8	ng	30703	1	6.834	223016	20.0
2-Pentanone, 4-...	5.063	10.3	ng	114630	1	6.834	223016	20.0
1-Phenoxypropan...	8.433	3.2	ng	46415	2	8.116	287930	20.0
unknown9.957	9.957	2.7	ng	43383	3	9.869	316373	20.0
Trifluoroacetox...	13.863	3.1	ng	25933	5	13.998	166436	20.0