LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130947.D
Acq On : 03 Nov 2022 00:23
Operator : CG\JU
Sample : N5380-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-C

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-BF102722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130947.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.216	15	22	30	rVB	445008	576603	35.08%	5.060%
2	2.328	36	41	47	rBV	35763	47139	2.87%	0.414%
3	5.146	515	520	527	rBV	253767	280480	17.07%	2.461%
4	5.540	582	587	590	rBV	1834425	1643560	100.00%	14.422%
5	6.545	752	758	770	rVB	1508611	1585699	96.48%	13.914%
6	6.922	818	822	825	rBV	429830	324221	19.73%	2.845%
7	7.487	913	918	921	rBV	1154921	983515	59.84%	8.630%
8	8.116	1020	1025	1034	rBV4	18585	50448	3.07%	0.443%
9	8.204	1037	1040	1044	rVB	411074	360532	21.94%	3.164%
10	9.286	1219	1224	1227	rBV	1647038	1428657	86.92%	12.536%
11	9.969	1336	1340	1343	rVB	391184	325711	19.82%	2.858%
12	10.757	1470	1474	1477	rBV	1014349	825039	50.20%	7.240%
13	11.457	1590	1593	1597	rBV	379734	322997	19.65%	2.834%
14	11.975	1678	1681	1685	rBV	37612	35346	2.15%	0.310%
15	13.051	1860	1864	1867	rBV	1691694	1422963	86.58%	12.486%
16	13.945	2014	2016	2018	rBV	23738	20473	1.25%	0.180%
17	14.033	2028	2031	2040	rVB9	40001	105366	6.41%	0.925%
18	14.110	2040	2044	2047	rVB	449227	396454	24.12%	3.479%
19	14.263	2068	2070	2074	rVB	16910	17913	1.09%	0.157%
20	14.574	2120	2123	2125	rBV3	26221	28699	1.75%	0.252%
21	14.874	2170	2174	2182	rBV	181546	232619	14.15%	2.041%
22	15.621	2296	2301	2309	rBV	290968	381882	23.24%	3.351%

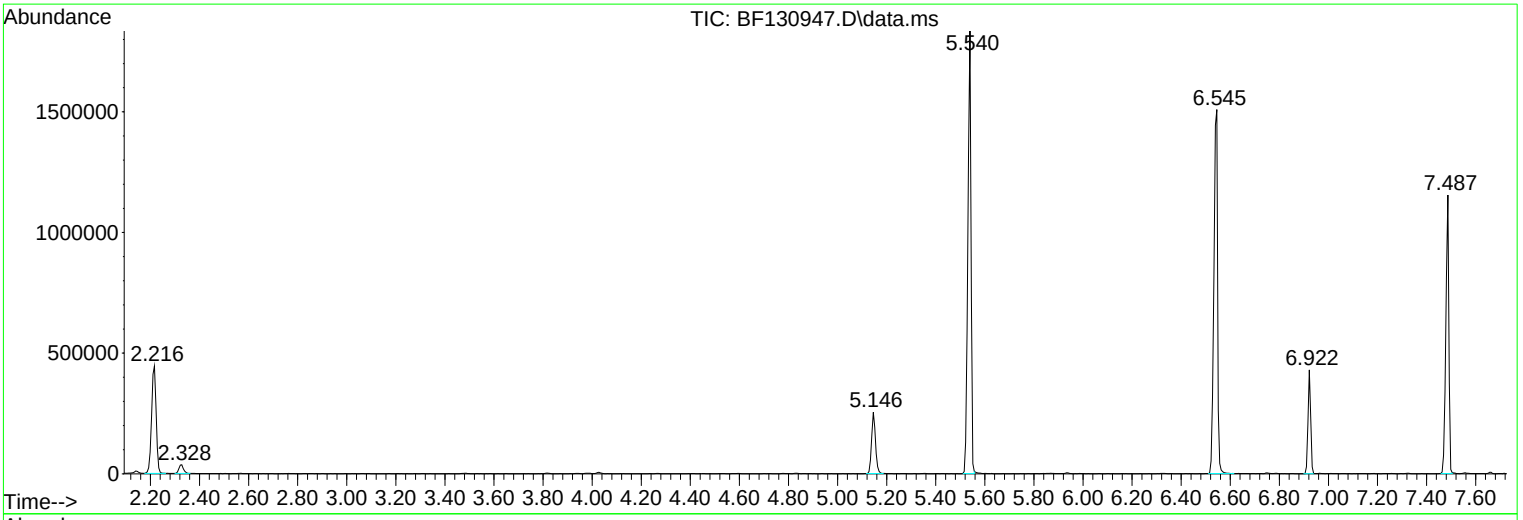
Sum of corrected areas: 11396316

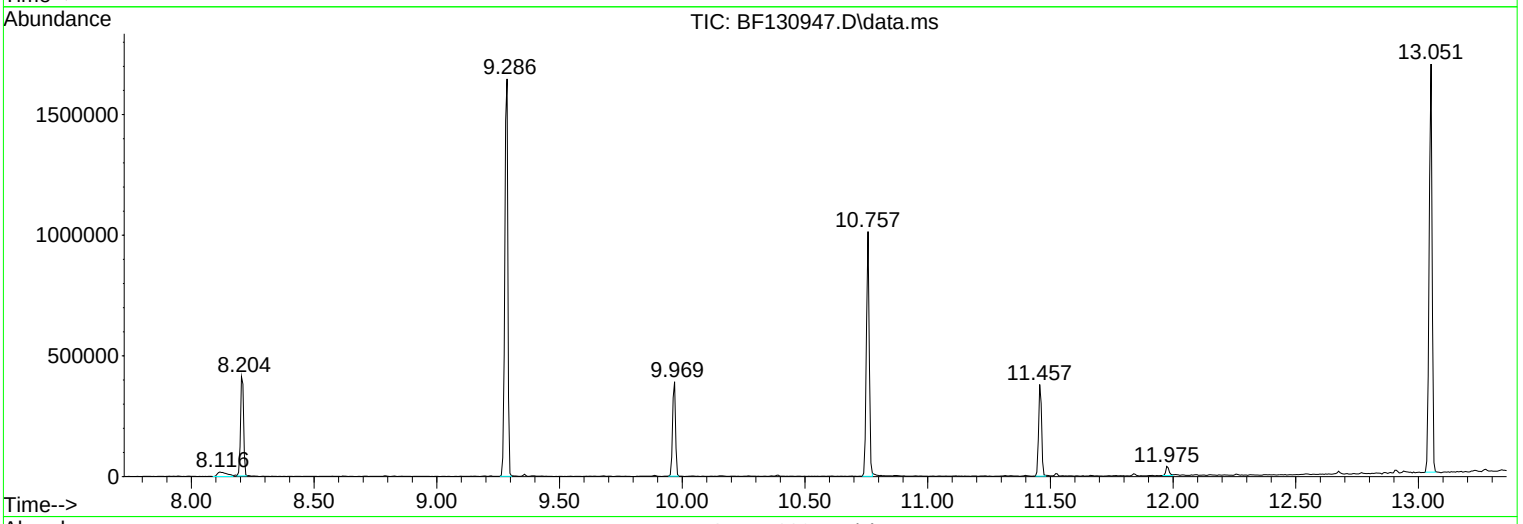
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130947.D
Acq On : 03 Nov 2022 00:23
Operator : CG\JU
Sample : N5380-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

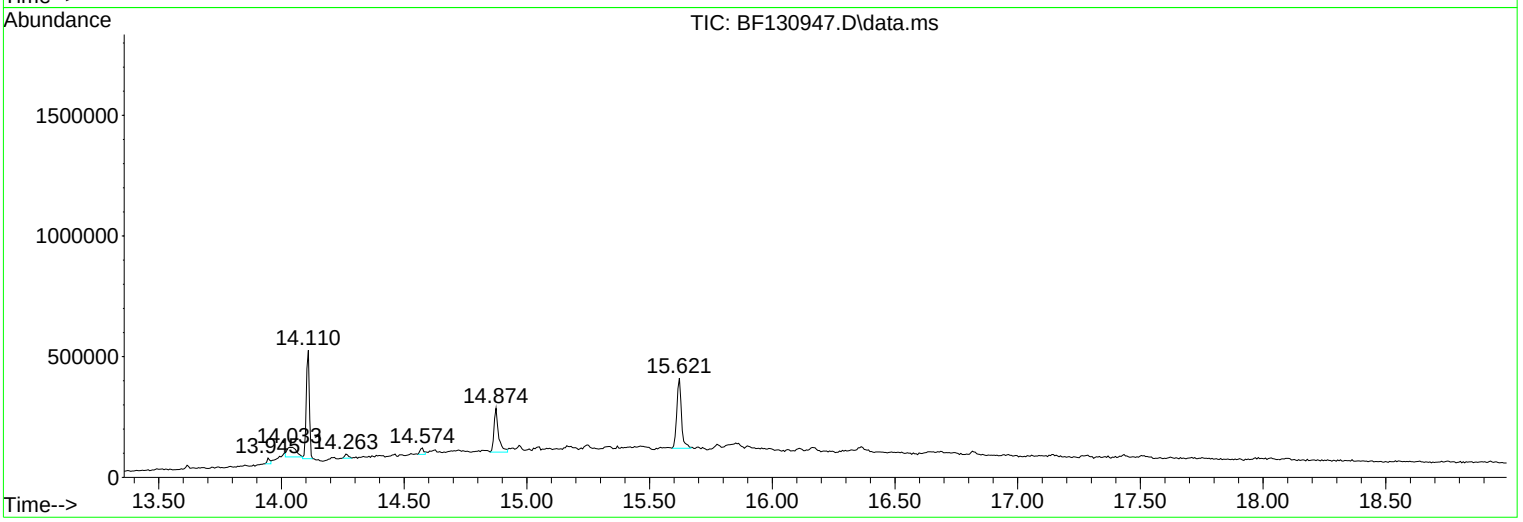
Instrument :
BNA_F
ClientSampleId :
TP-C

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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\BF110222\
Data File : BF130947.D
Acq On : 03 Nov 2022 00:23
Operator : CG\JU
Sample : N5380-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-C

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

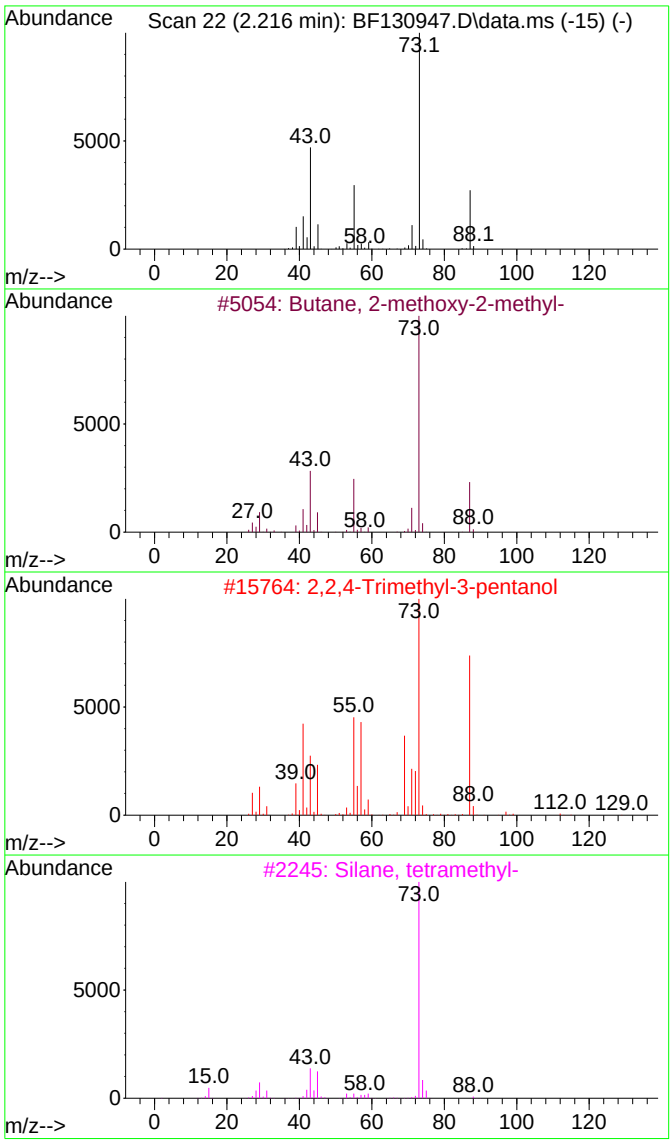
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

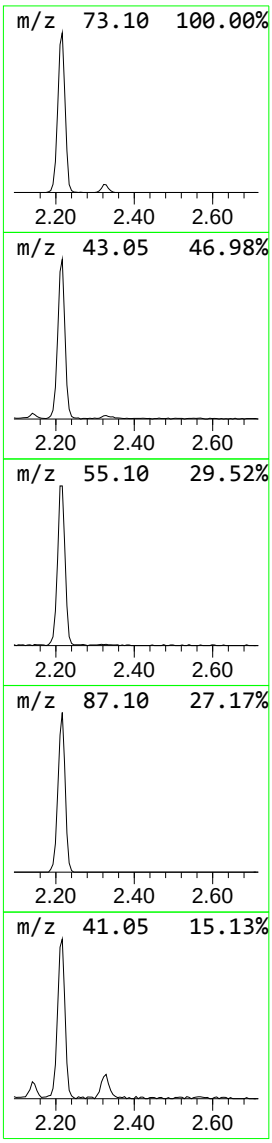
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.216	35.57 ng	576603	1,4-Dichlorobenzene-d4	6.922

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	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130947.D
Acq On : 03 Nov 2022 00:23
Operator : CG\JU
Sample : N5380-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-C

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

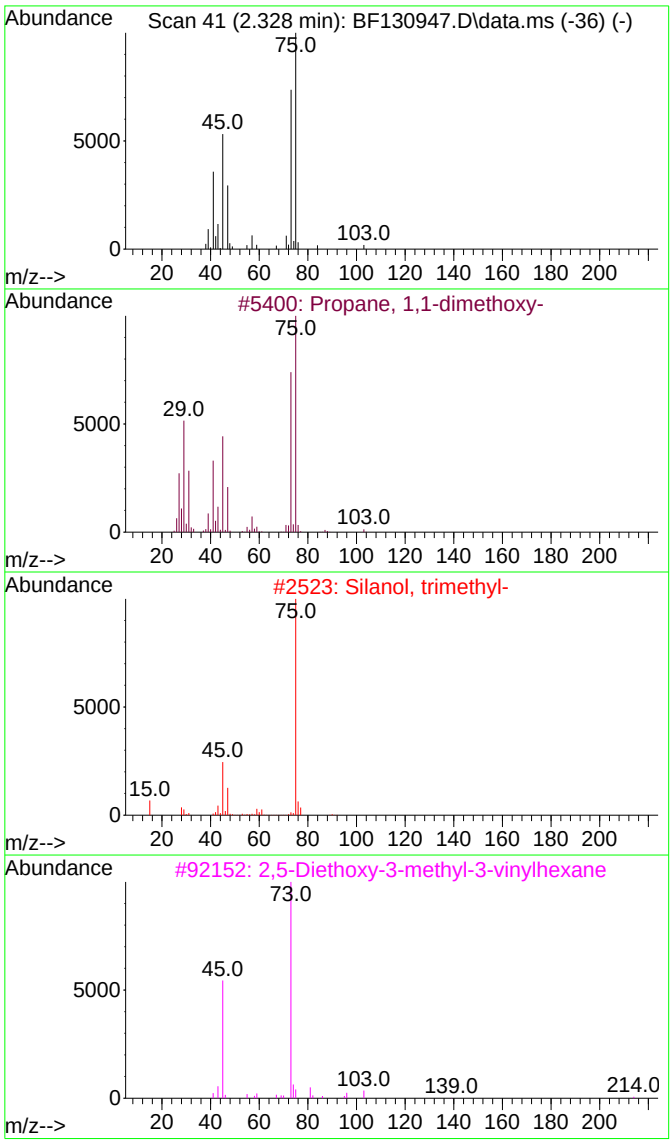
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

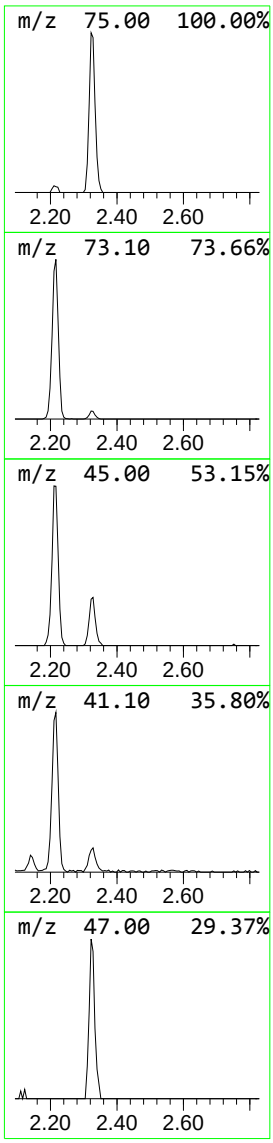
****

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.328	2.91 ng	47139	1,4-Dichlorobenzene-d4	6.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	74
2	Silanol, trimethyl-	90	C3H10OSi	001066-40-6	64
3	2,5-Diethoxy-3-methyl-3-vinylhexane	214	C13H26O2	1000432-70-8	9
4	1-Butyne, 4,4-dimethoxy-	114	C6H10O2	033639-45-1	9
5	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130947.D
Acq On : 03 Nov 2022 00:23
Operator : CG\JU
Sample : N5380-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-C

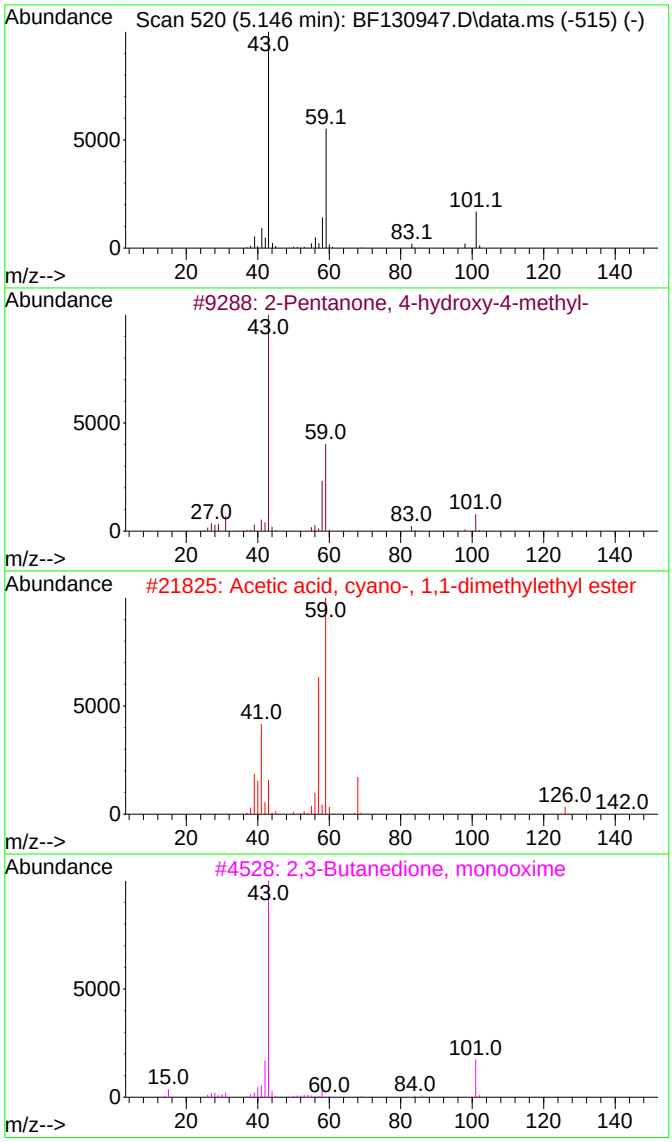
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

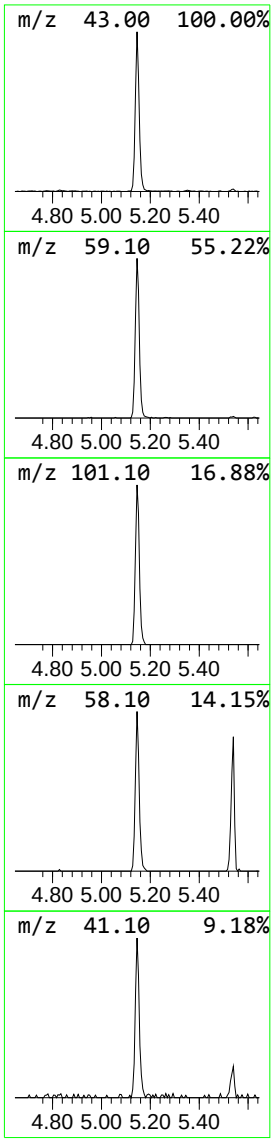
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.146	17.30 ng	280480	1,4-Dichlorobenzene-d4	6.922

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	25
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130947.D
Acq On : 03 Nov 2022 00:23
Operator : CG\JU
Sample : N5380-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-C

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

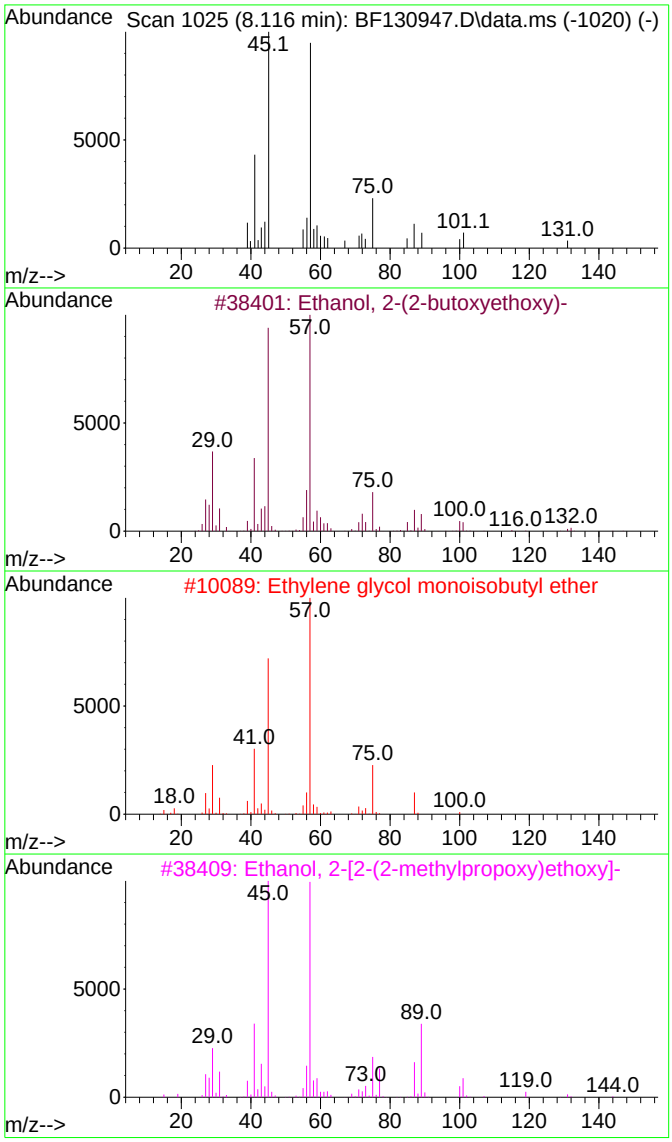
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

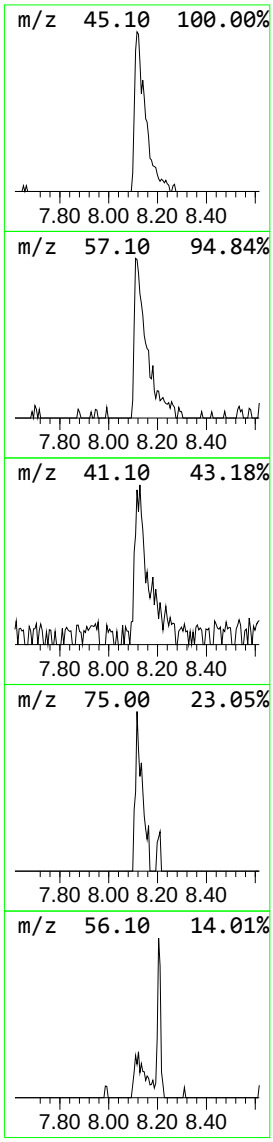
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.116	2.80 ng	50448	Naphthalene-d8	8.204

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	86
2	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
4	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	45
5	Ethylene glycol diglycidyl ether	174	C8H14O4	002224-15-9	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130947.D
Acq On : 03 Nov 2022 00:23
Operator : CG\JU
Sample : N5380-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-C

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

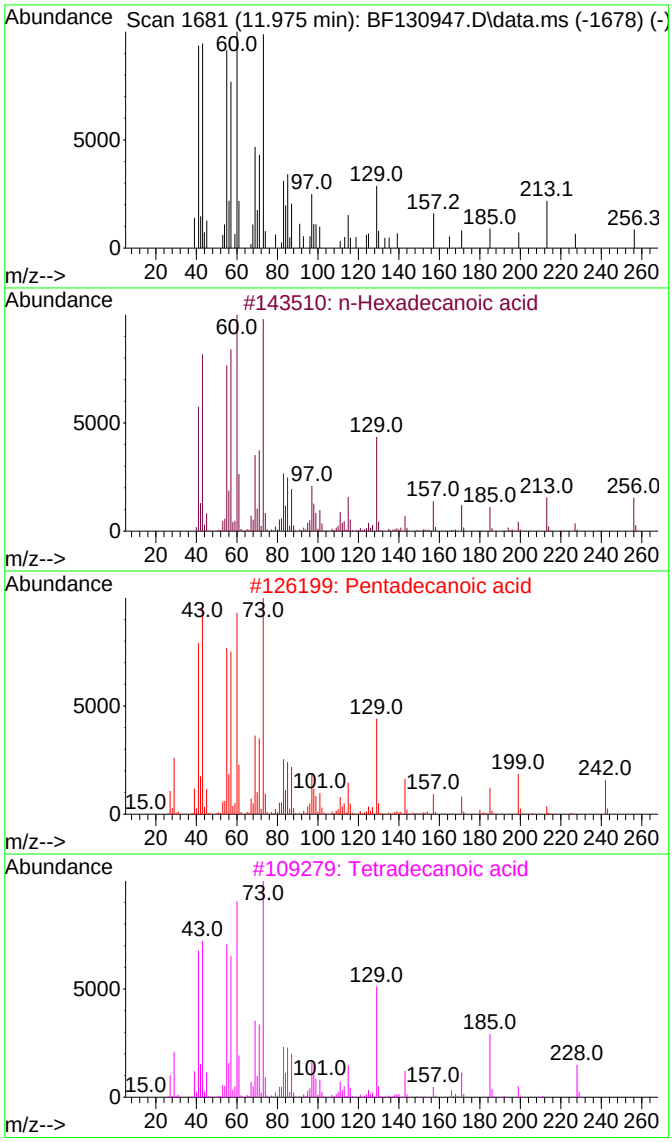
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

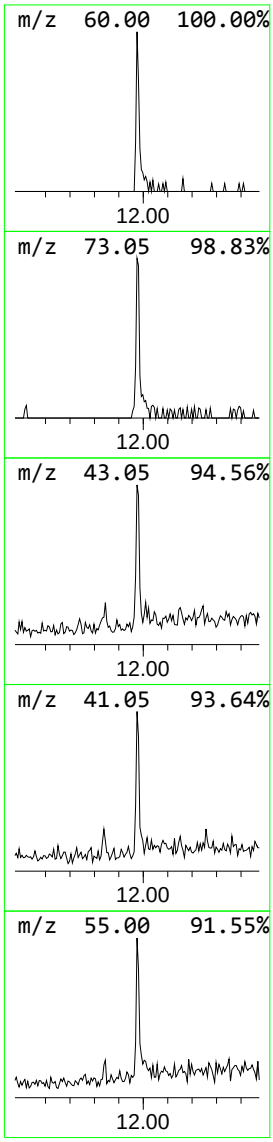
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.975	2.19 ng	35346	Phenanthrene-d10	11.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	92
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Undecanoic acid	186	C11H22O2	000112-37-8	64
5	Tridecanoic acid	214	C13H26O2	000638-53-9	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130947.D
Acq On : 03 Nov 2022 00:23
Operator : CG\JU
Sample : N5380-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-C

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

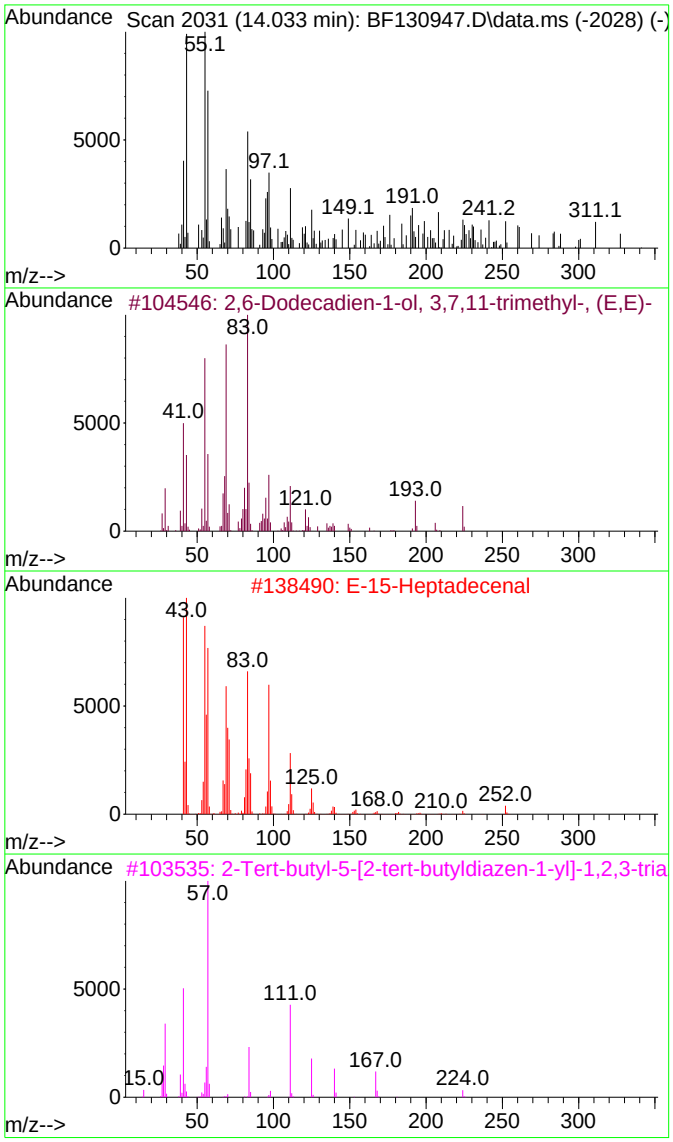
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

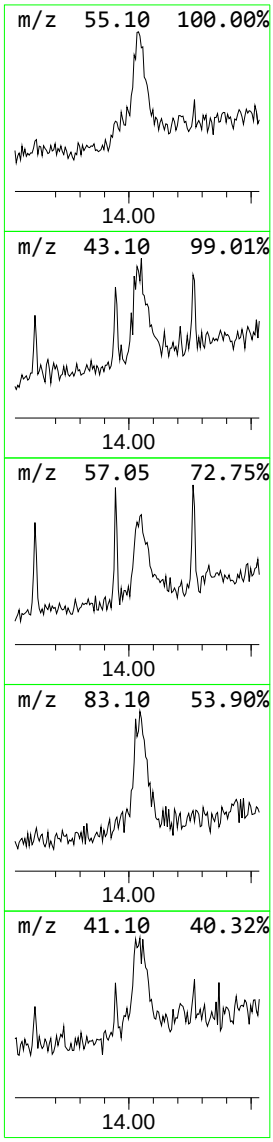
****

Peak Number 6 unknown14.033 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.033	5.32 ng	105366	Chrysene-d12	14.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6-Dodecadien-1-ol, 3,7,11-trim...	224	C15H28O	020576-56-1	15
2	E-15-Heptadecenal	252	C17H32O	1000130-97-9	11
3	2-Tert-butyl-5-[2-tert-butyldiaz...	224	C10H20N6	1000411-43-5	10
4	3-Chloropropionic acid, octadecy...	360	C21H41ClO2	088168-99-4	10
5	E-7-Octadecene	252	C18H36	1000130-92-0	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130947.D
Acq On : 03 Nov 2022 00:23
Operator : CG\JU
Sample : N5380-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-C

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

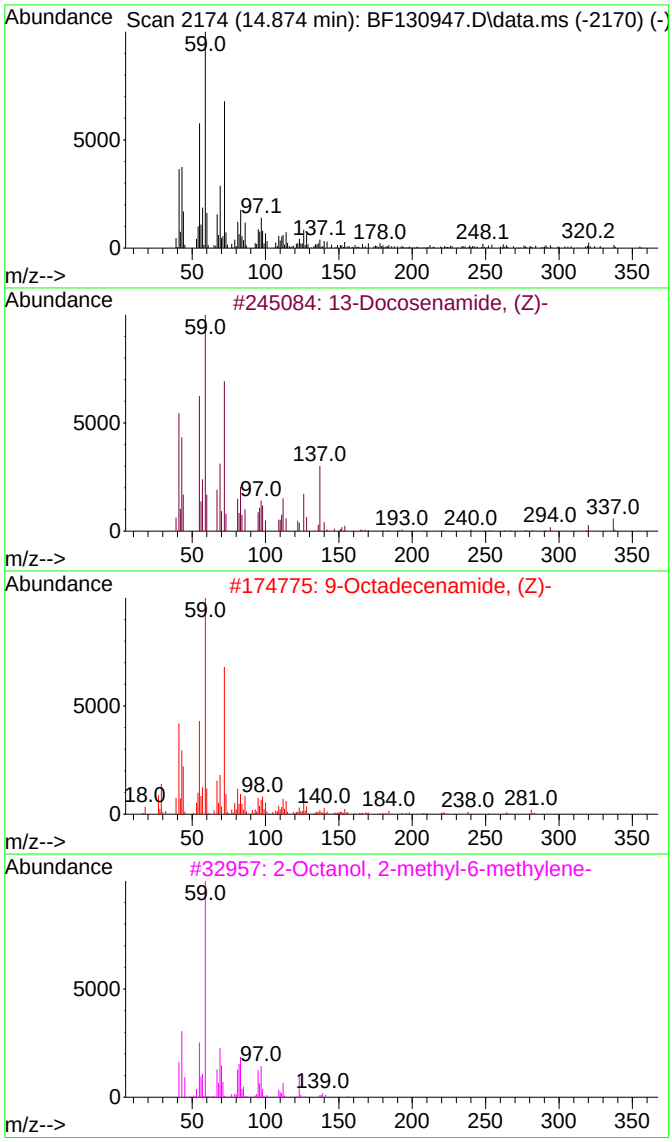
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

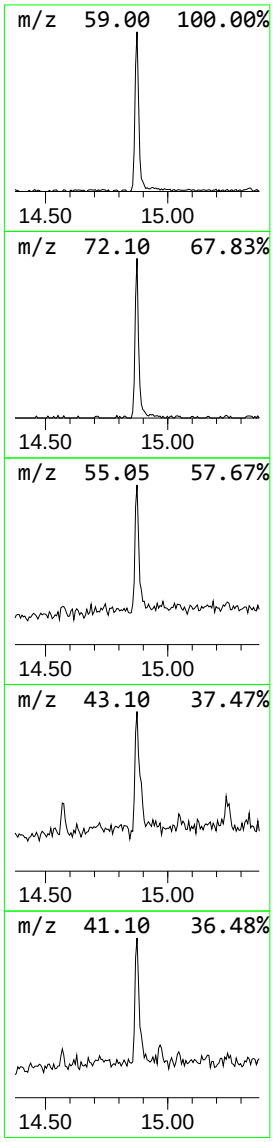
****

Peak Number 7 13-Docosenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.874	12.18 ng	232619	Perylene-d12	15.621

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	93
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
3	2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	49
4	2-Hydroxy-2,4-dimethyl-hept-6-en...	156	C9H16O2	1000192-56-0	38
5	2-Propenoic acid	72	C3H4O2	000079-10-7	11





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130947.D
Acq On : 03 Nov 2022 00:23
Operator : CG\JU
Sample : N5380-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-C

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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...	2.216	35.6	ng	576603	1	6.922	324221	20.0
Propane, 1,1-di...	2.328	2.9	ng	47139	1	6.922	324221	20.0
2-Pentanone, 4-...	5.146	17.3	ng	280480	1	6.922	324221	20.0
Ethanol, 2-(2-b...	8.116	2.8	ng	50448	2	8.204	360532	20.0
n-Hexadecanoic ...	11.975	2.2	ng	35346	4	11.457	322997	20.0
unknown14.033	14.033	5.3	ng	105366	5	14.110	396454	20.0
13-Docosenamide...	14.874	12.2	ng	232619	6	15.621	381882	20.0