LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061024\
Data File : BF138173.D
Acq On : 10 Jun 2024 15:42
Operator : CG\JU
Sample : P2795-07
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-3-(10-15)-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-BF060524.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138173.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.204	12	20	26	rBV	5637874	7330888	79.14%	10.764%
2	3.422	222	227	242	rBV	149071	294398	3.18%	0.432%
3	5.122	512	516	525	rVB	329437	395014	4.26%	0.580%
4	5.516	578	583	586	rBV	7562847	7352025	79.37%	10.795%
5	6.522	748	754	757	rBV	7003767	7436418	80.28%	10.919%
6	6.716	784	787	793	rBV	165888	158118	1.71%	0.232%
7	6.898	814	818	821	rVB	2593035	2177947	23.51%	3.198%
8	7.457	908	913	916	rBV	5317291	4444542	47.98%	6.526%
9	8.175	1031	1035	1039	rBV	3453019	2922078	31.55%	4.291%
10	8.486	1084	1088	1099	rBV	153493	187597	2.03%	0.275%
11	9.251	1214	1218	1222	rBV	9793388	9262653	100.00%	13.601%
12	9.933	1330	1334	1337	rVB	3938746	3291383	35.53%	4.833%
13	10.033	1345	1351	1364	rBV	2274738	3034611	32.76%	4.456%
14	10.722	1463	1468	1471	rBV	4745208	4381529	47.30%	6.434%
15	11.416	1582	1586	1590	rBV	3843009	3095698	33.42%	4.546%
16	11.945	1668	1676	1680	rBV	332037	348202	3.76%	0.511%
17	12.727	1805	1809	1820	rVB	139250	132575	1.43%	0.195%
18	13.004	1852	1856	1859	rBV	8910304	7608402	82.14%	11.172%
19	13.910	2007	2010	2013	rBV	87836	104794	1.13%	0.154%
20	14.051	2030	2034	2043	rBV	2379966	2057600	22.21%	3.021%
21	14.921	2178	2182	2188	rBV	208785	209809	2.27%	0.308%
22	15.533	2280	2286	2292	rBV	1506868	1877044	20.26%	2.756%

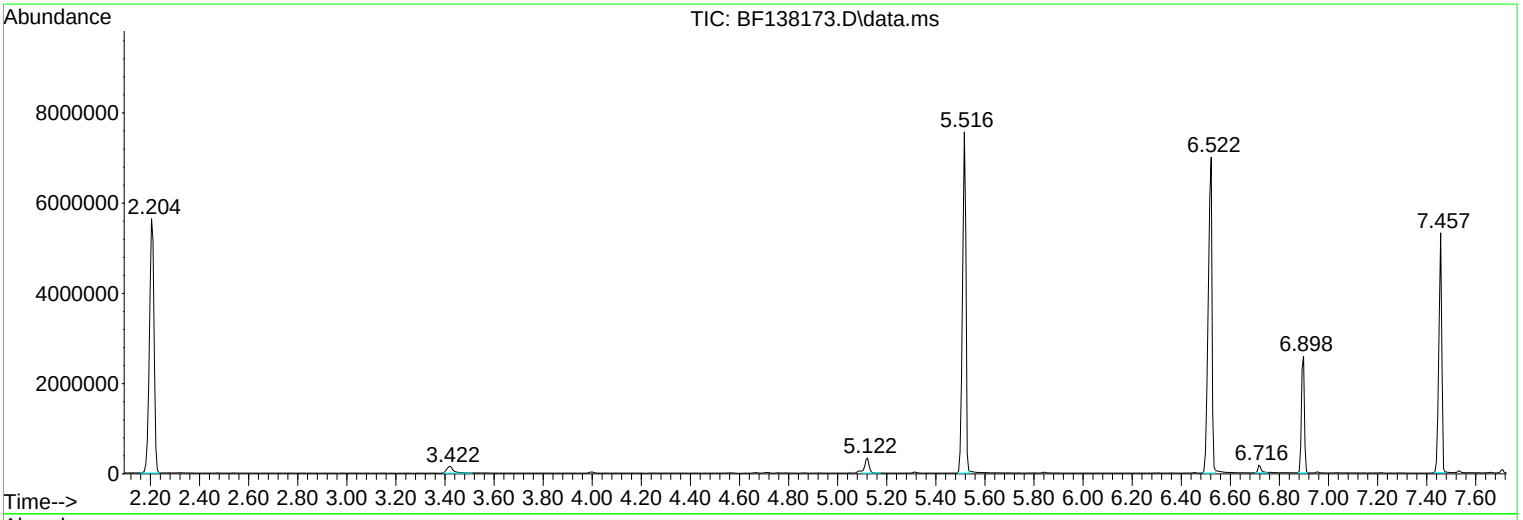
Sum of corrected areas: 68103325

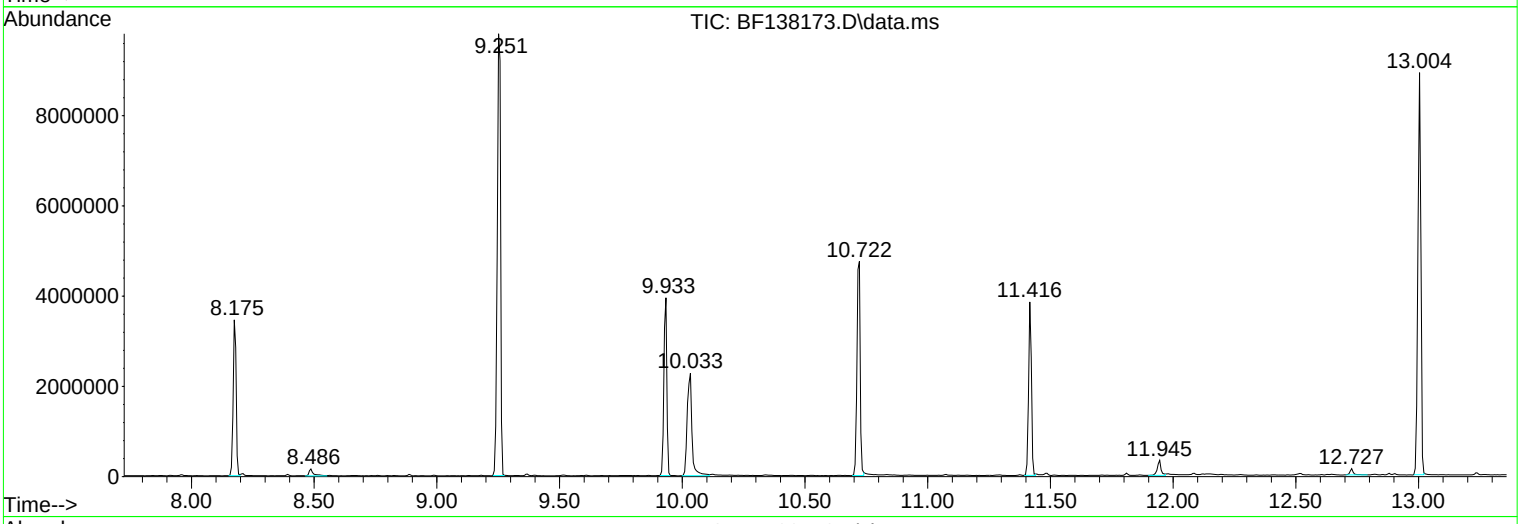
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061024\
Data File : BF138173.D
Acq On : 10 Jun 2024 15:42
Operator : CG\JU
Sample : P2795-07
Misc :
ALS Vial : 4 Sample Multiplier: 1

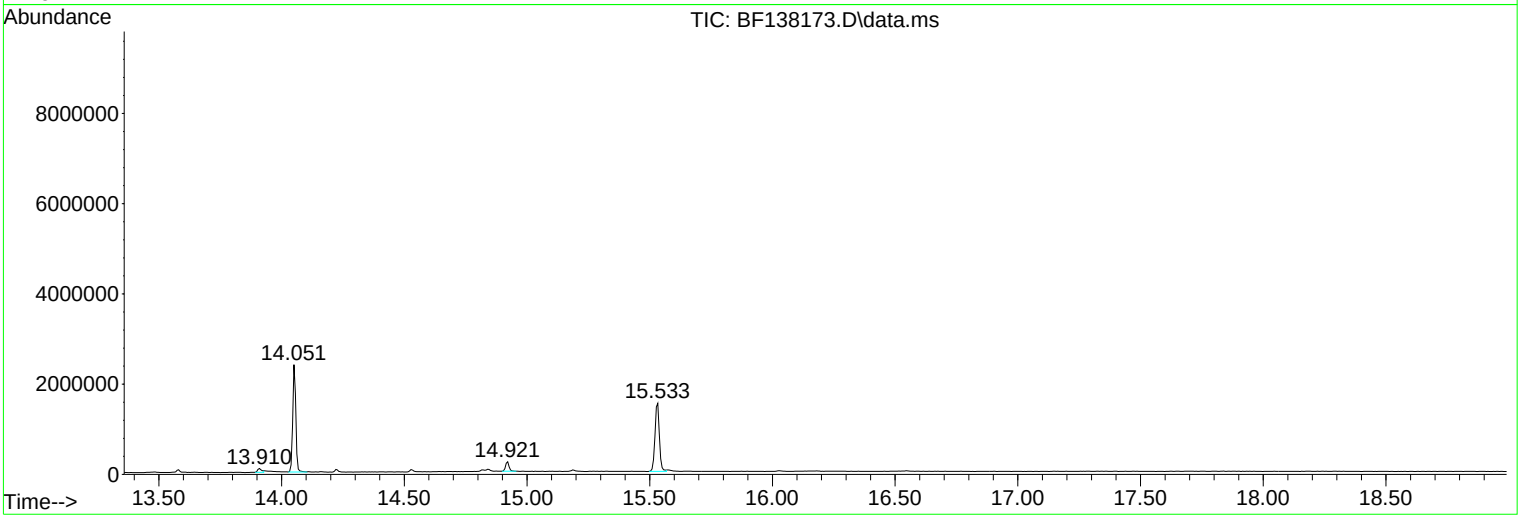
Instrument :
BNA_F
ClientSampleId :
WC-3-(10-15)-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060524.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\BF061024\
Data File : BF138173.D
Acq On : 10 Jun 2024 15:42
Operator : CG\JU
Sample : P2795-07
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-3-(10-15)-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

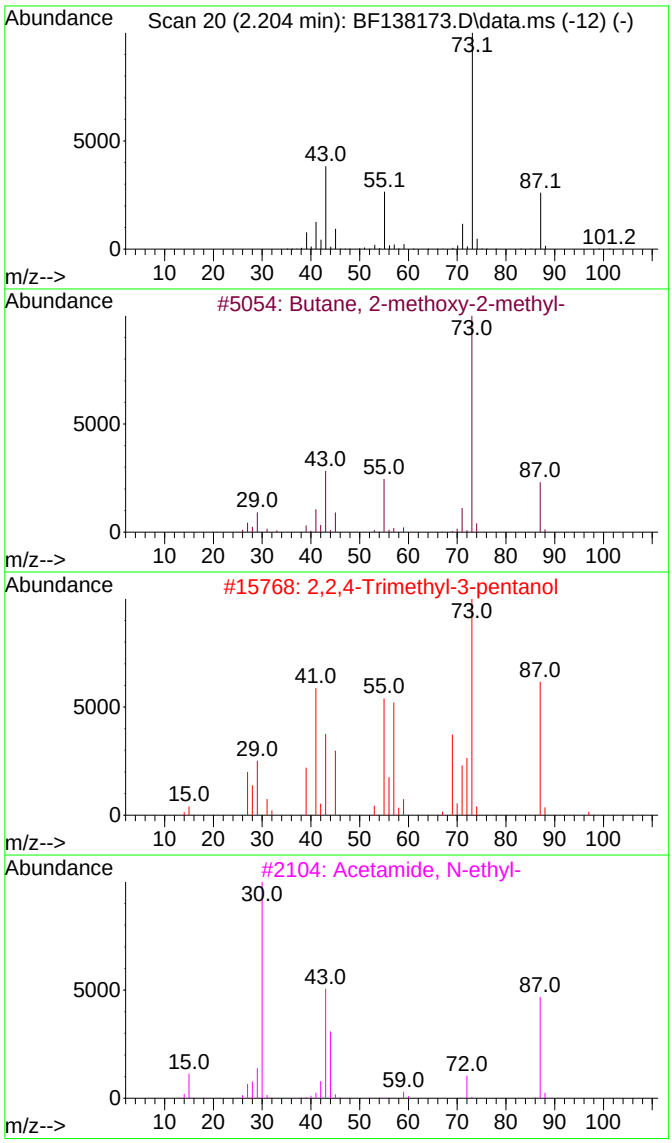
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

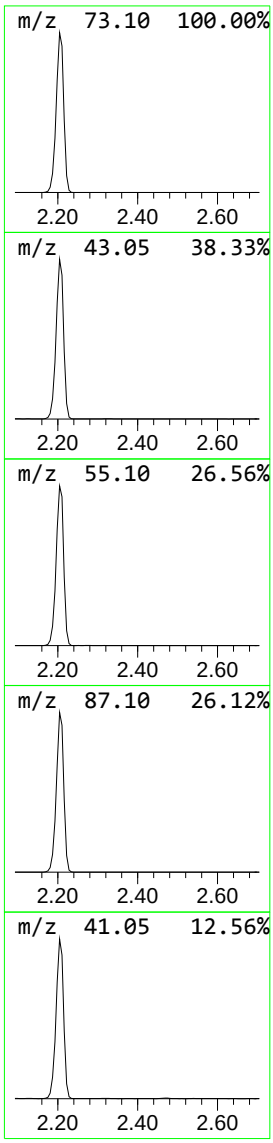
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.204	67.32 ng	7330890	1,4-Dichlorobenzene-d4	6.898

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	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061024\
Data File : BF138173.D
Acq On : 10 Jun 2024 15:42
Operator : CG\JU
Sample : P2795-07
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-3-(10-15)-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

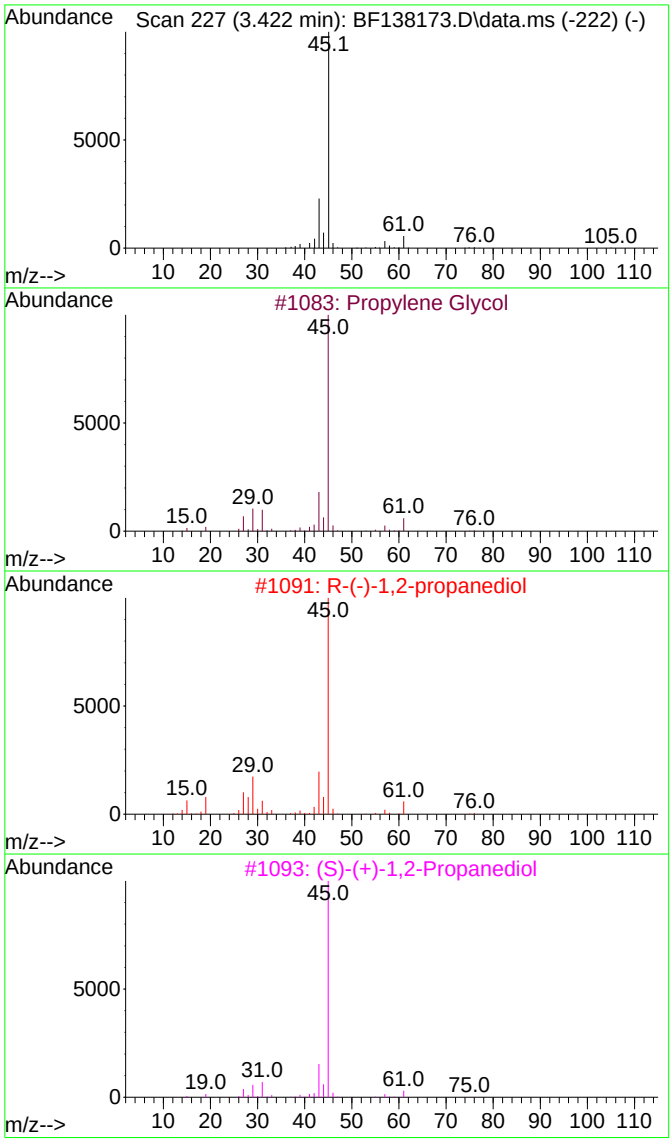
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

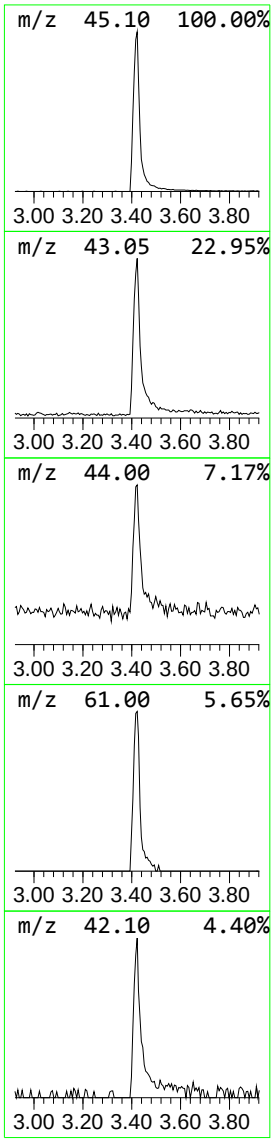
****

Peak Number 2 Propylene Glycol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.422	2.70 ng	294398	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	90
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	78
3	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40
4	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
5	Butanenitrile, 2-(methoxymethoxy)	129	C6H11NO2	1000196-86-5	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061024\
Data File : BF138173.D
Acq On : 10 Jun 2024 15:42
Operator : CG\JU
Sample : P2795-07
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-3-(10-15)-COMP

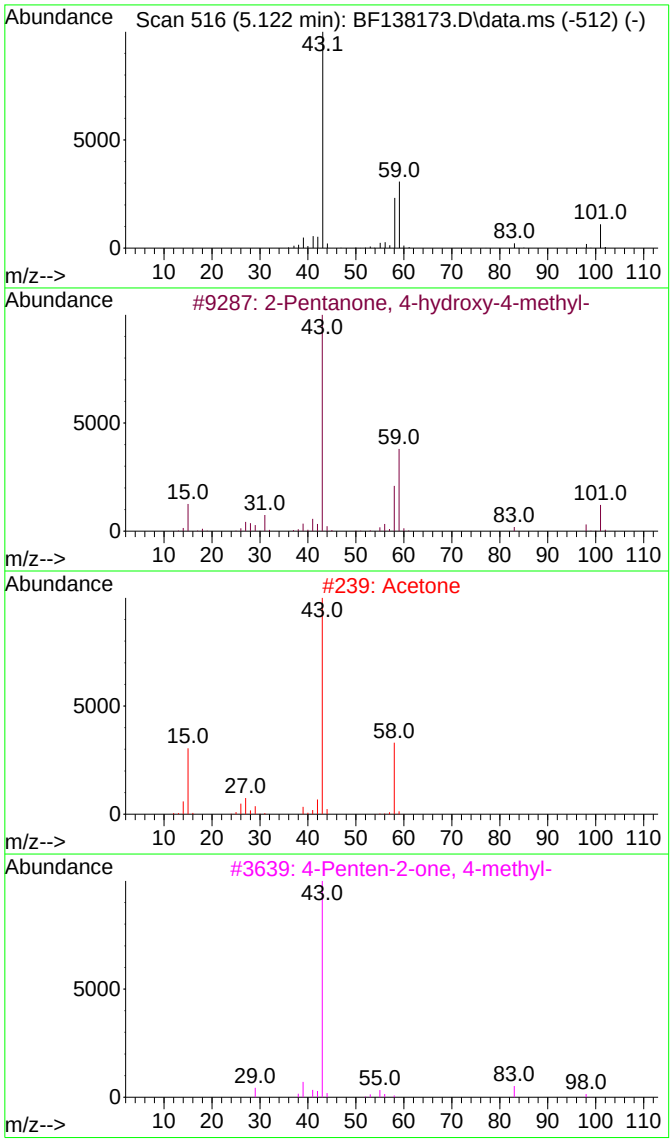
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

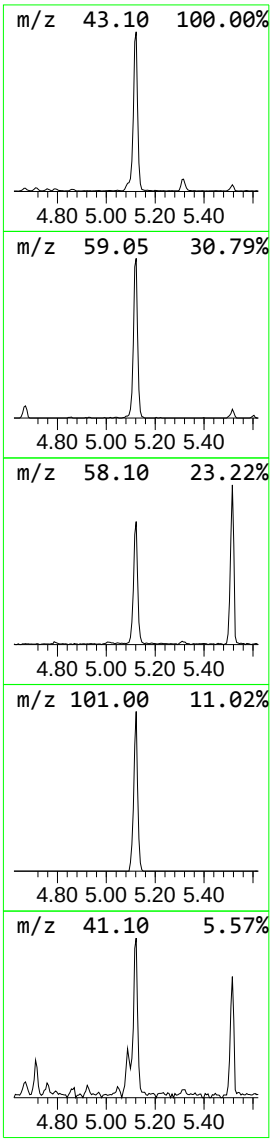
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.122	3.63 ng	395014	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	78
2	Acetone	58	C3H6O	000067-64-1	32
3	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	10
4	Propylamine	59	C3H9N	000107-10-8	9
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061024\
Data File : BF138173.D
Acq On : 10 Jun 2024 15:42
Operator : CG\JU
Sample : P2795-07
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-3-(10-15)-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

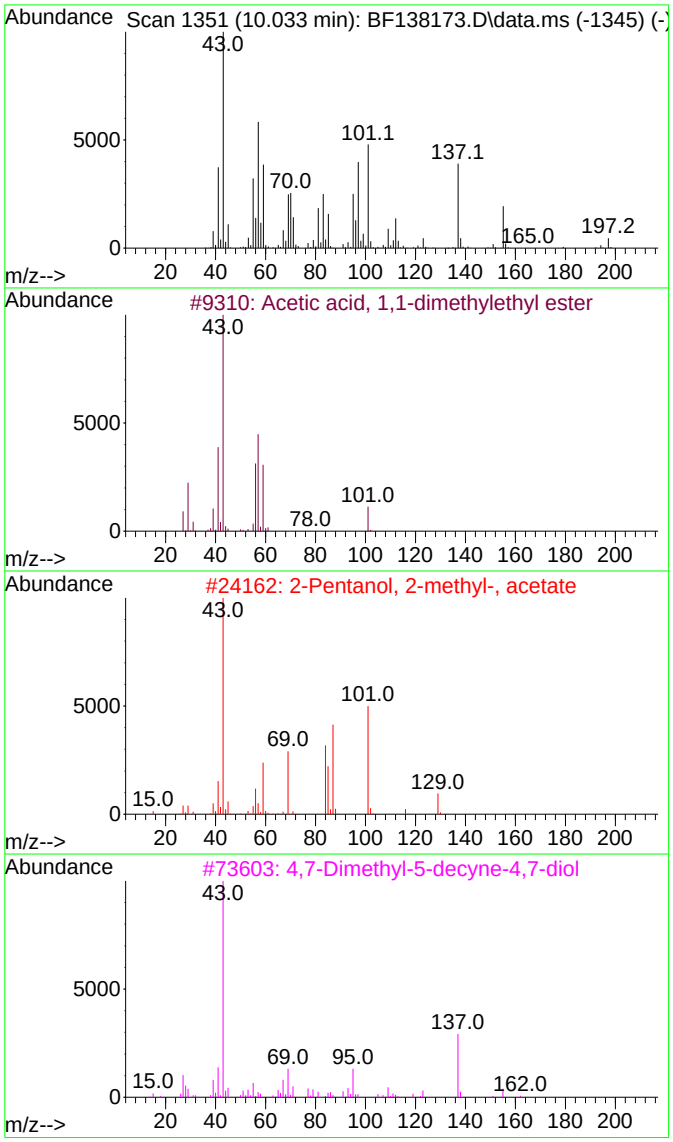
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

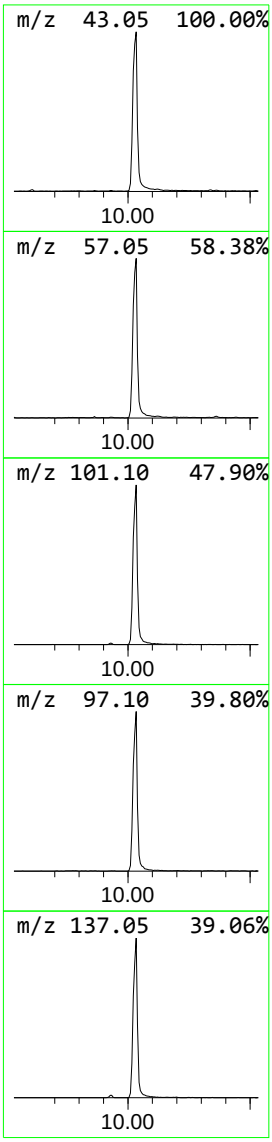
****

Peak Number 4 unknown10.033 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.033	18.44 ng	3034610	Acenaphthene-d10	9.933

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	14
2	2-Pentanol, 2-methyl-, acetate	144	C8H16O2	034859-98-8	10
3	4,7-Dimethyl-5-decyne-4,7-diol	198	C12H22O2	000126-87-4	10
4	Pentadecane, 1-bromo-	290	C15H31Br	000629-72-1	10
5	Pent-4-enoyl amide, 2-methyl-N-p...	155	C9H17NO	1000420-35-2	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061024\
Data File : BF138173.D
Acq On : 10 Jun 2024 15:42
Operator : CG\JU
Sample : P2795-07
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-3-(10-15)-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

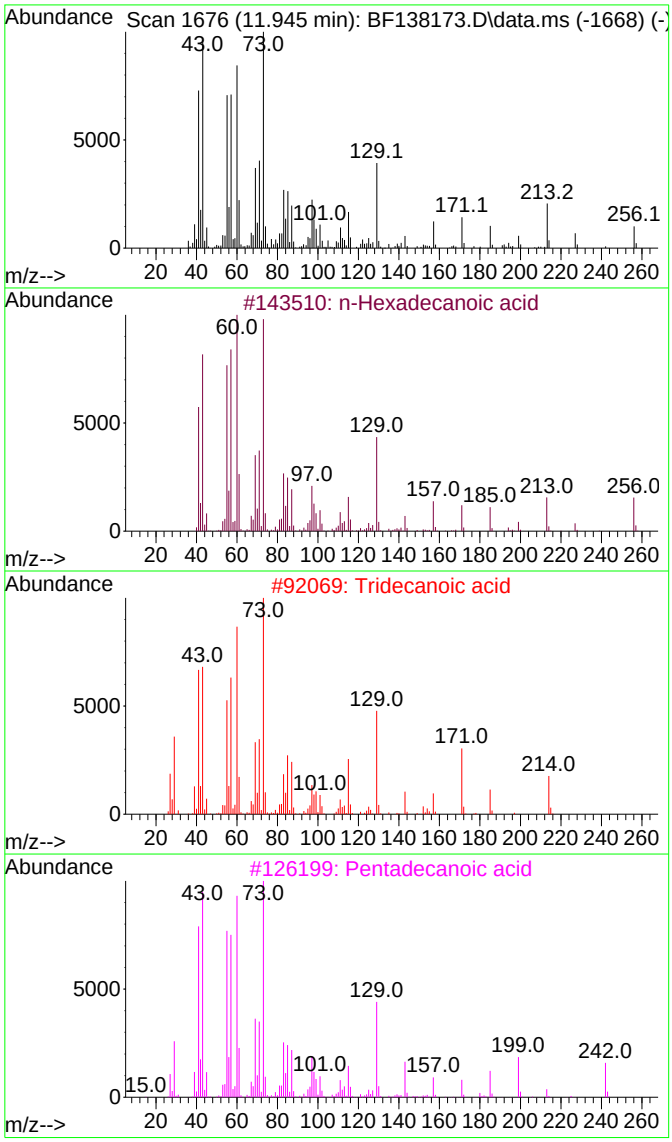
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

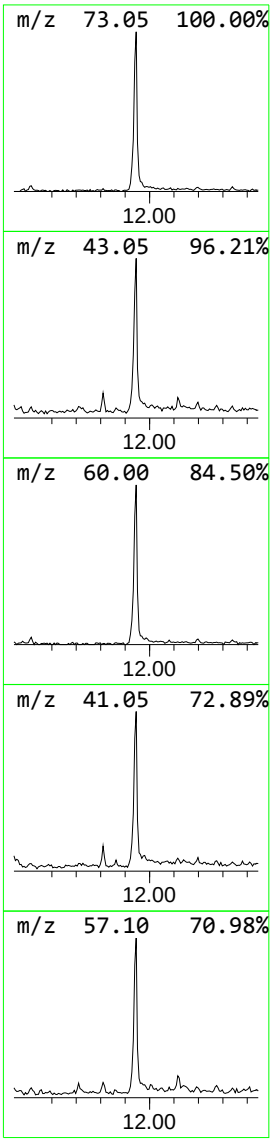
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	2.25 ng	348202	Phenanthrene-d10	11.416

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	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061024\
Data File : BF138173.D
Acq On : 10 Jun 2024 15:42
Operator : CG\JU
Sample : P2795-07
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-3-(10-15)-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

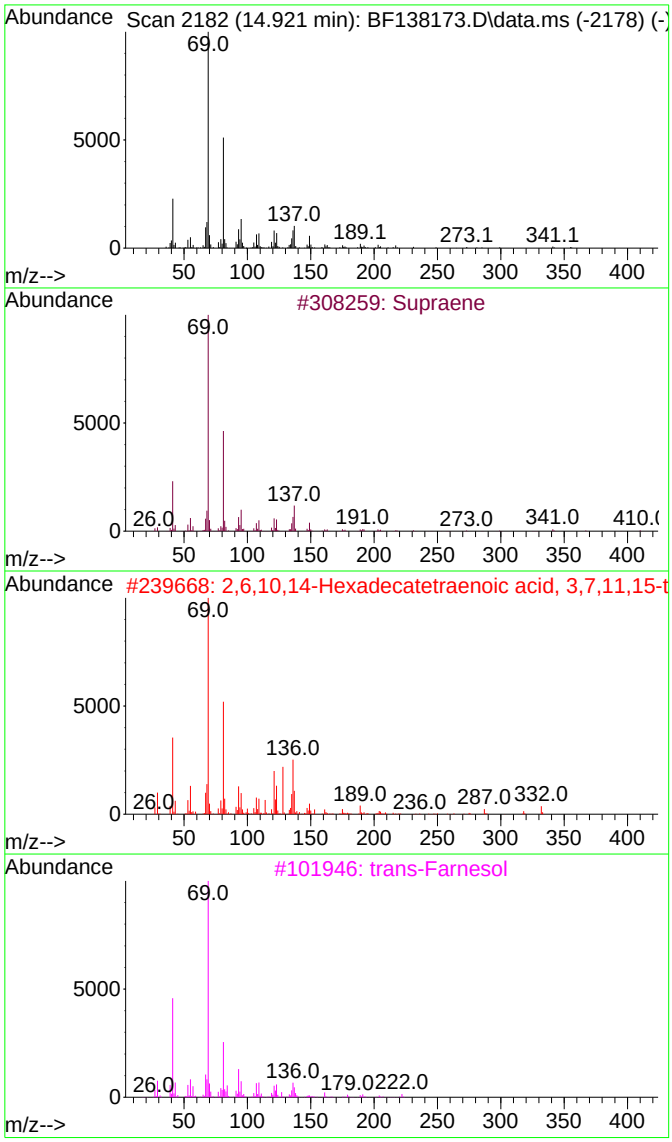
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

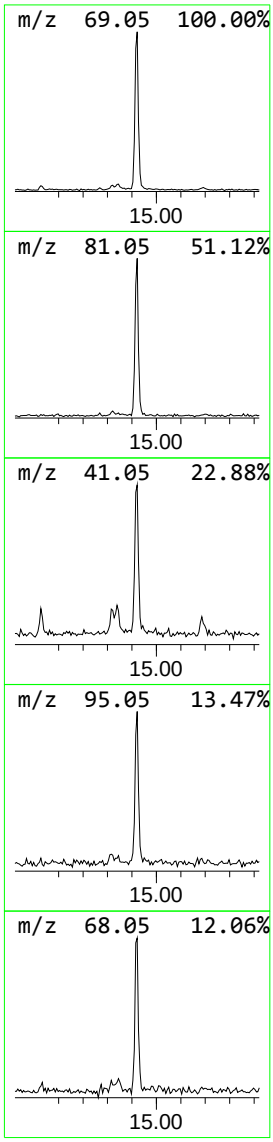
****

Peak Number 6 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.921	2.24 ng	209809	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
3	trans-Farnesol	222	C15H26O	000106-28-5	72
4	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
5	3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061024\
Data File : BF138173.D
Acq On : 10 Jun 2024 15:42
Operator : CG\JU
Sample : P2795-07
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-3-(10-15)-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060524.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...	2.204	67.3	ng	7330890	1	6.898	2177950	20.0
Propylene Glycol	3.422	2.7	ng	294398	1	6.898	2177950	20.0
2-Pentanone, 4-...	5.122	3.6	ng	395014	1	6.898	2177950	20.0
unknown10.033	10.033	18.4	ng	3034610	3	9.933	3291380	20.0
n-Hexadecanoic ...	11.945	2.3	ng	348202	4	11.416	3095700	20.0
Supraene	14.921	2.2	ng	209809	6	15.533	1877040	20.0