LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071124\
Data File : BF138530.D
Acq On : 11 Jul 2024 18:48
Operator : CG\JU
Sample : P3187-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-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-BF070924.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138530.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	6	14	19	rBV	1565345	2060090	84.20%	11.700%
2	3.392	220	222	233	rBV	20151	48542	1.98%	0.276%
3	5.086	506	510	517	rVB	145376	163923	6.70%	0.931%
4	5.492	574	579	582	rBV	2213903	2038107	83.30%	11.575%
5	6.498	745	750	753	rBV	2235624	2124169	86.82%	12.063%
6	6.863	808	812	815	rBV	704914	564669	23.08%	3.207%
7	7.422	902	907	910	rBV	1396769	1403000	57.34%	7.968%
8	7.827	971	976	979	rBV	39792	32858	1.34%	0.187%
9	8.139	1025	1029	1033	rBV	803654	741494	30.30%	4.211%
10	9.216	1207	1212	1215	rBV	2744518	2446773	100.00%	13.896%
11	9.898	1324	1328	1331	rBV	874079	788450	32.22%	4.478%
12	9.992	1339	1344	1349	rVB	65056	82091	3.36%	0.466%
13	10.686	1457	1462	1465	rBV	1318989	1260567	51.52%	7.159%
14	11.380	1576	1580	1583	rBV	875894	690104	28.20%	3.919%
15	11.904	1665	1669	1674	rBV	150342	144859	5.92%	0.823%
16	12.686	1800	1802	1810	rBV2	33130	38321	1.57%	0.218%
17	12.962	1845	1849	1853	rBV	2036966	1803053	73.69%	10.240%
18	13.862	1998	2002	2004	rBV2	34688	44867	1.83%	0.255%
19	14.015	2024	2028	2035	rVB	553914	478294	19.55%	2.716%
20	14.480	2103	2107	2111	rBV	32701	29777	1.22%	0.169%
21	14.768	2152	2156	2164	rBV2	157989	203660	8.32%	1.157%
22	15.480	2272	2277	2289	rVB	337848	420639	17.19%	2.389%

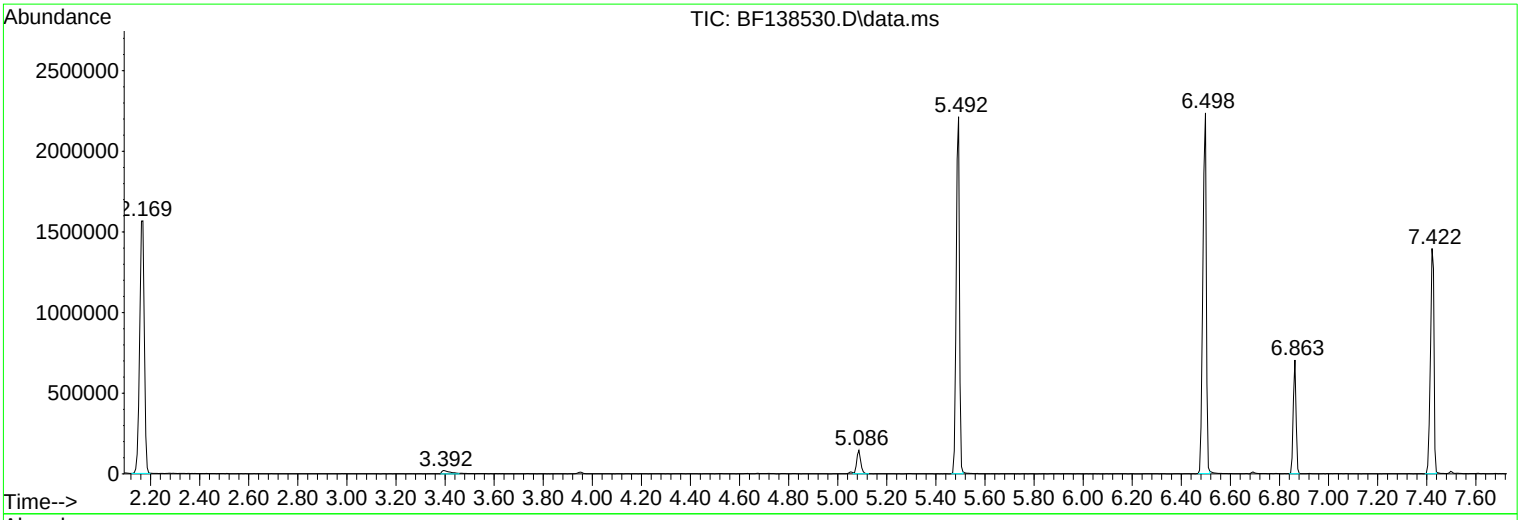
Sum of corrected areas: 17608307

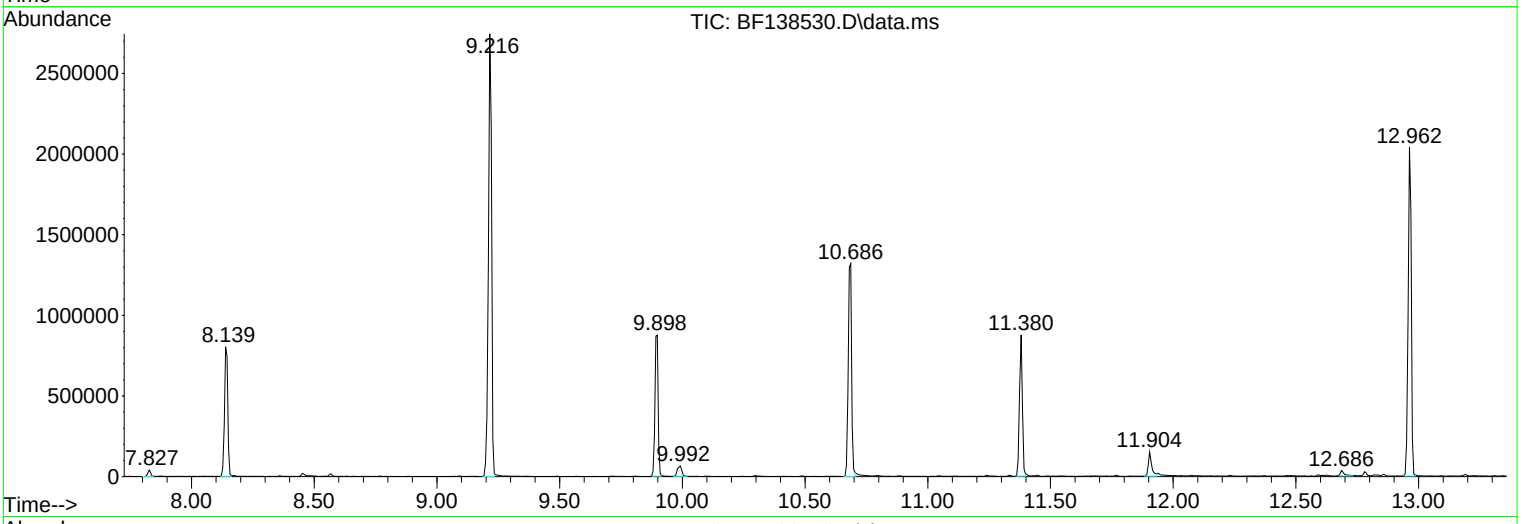
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071124\
Data File : BF138530.D
Acq On : 11 Jul 2024 18:48
Operator : CG\JU
Sample : P3187-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

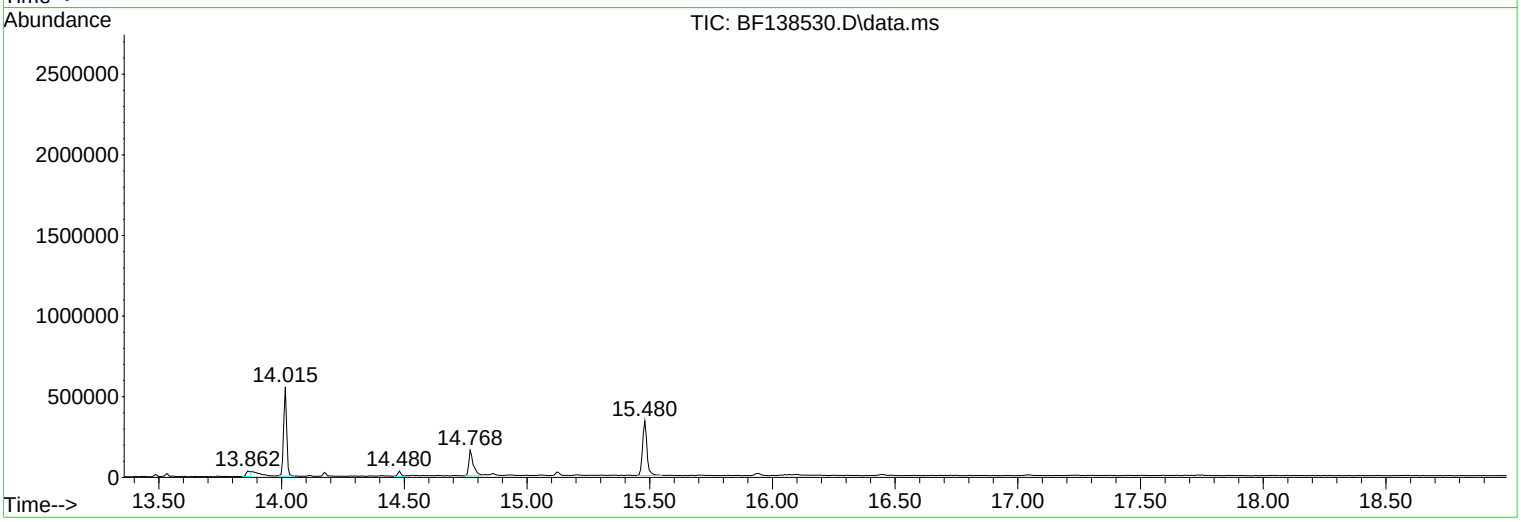
Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.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\BF071124\
Data File : BF138530.D
Acq On : 11 Jul 2024 18:48
Operator : CG\JU
Sample : P3187-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

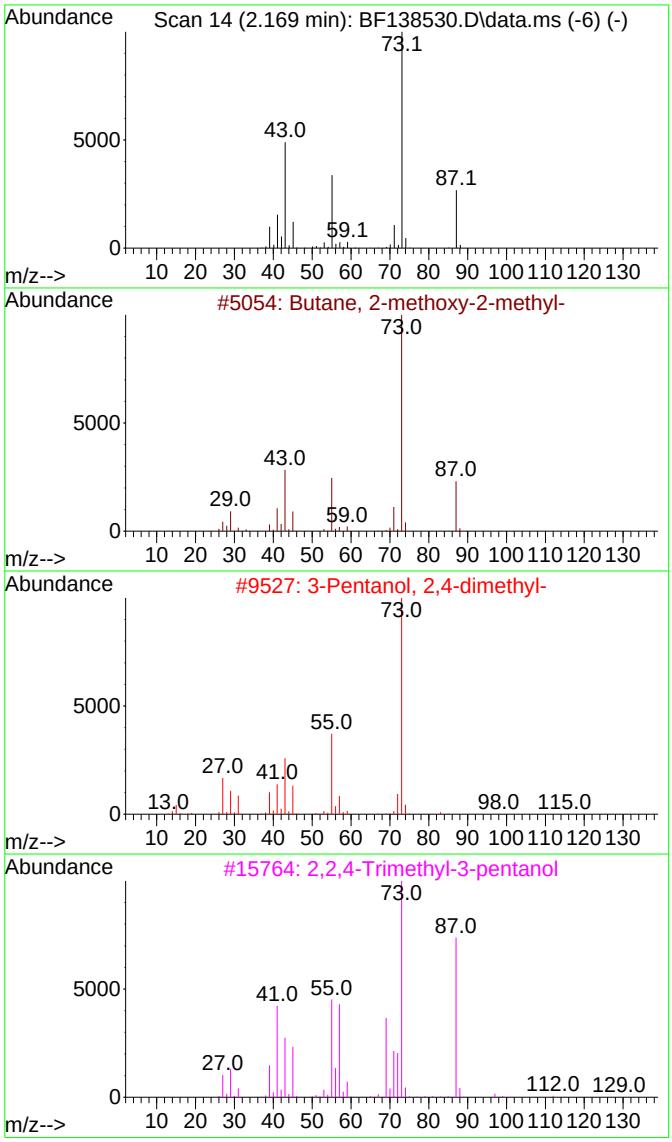
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

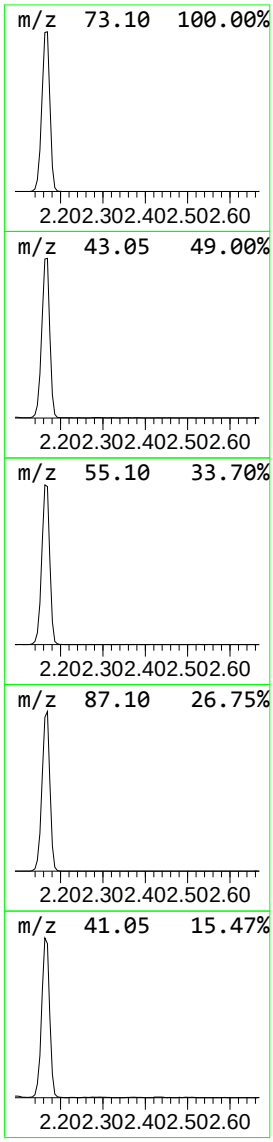
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	72.97 ng	2060090	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071124\
Data File : BF138530.D
Acq On : 11 Jul 2024 18:48
Operator : CG\JU
Sample : P3187-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

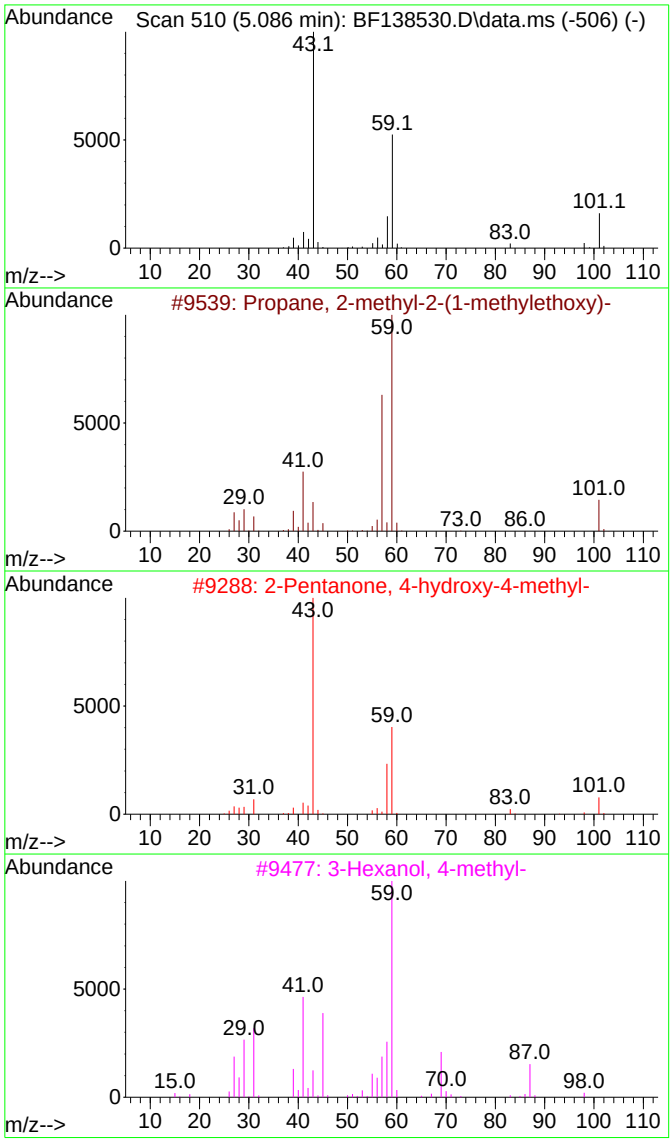
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

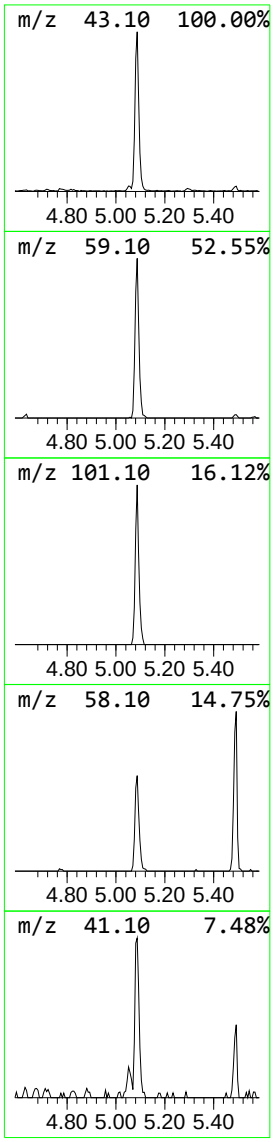
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Propane, 2-methyl-2-(1-meth... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.086	5.81 ng	163923	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071124\
Data File : BF138530.D
Acq On : 11 Jul 2024 18:48
Operator : CG\JU
Sample : P3187-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

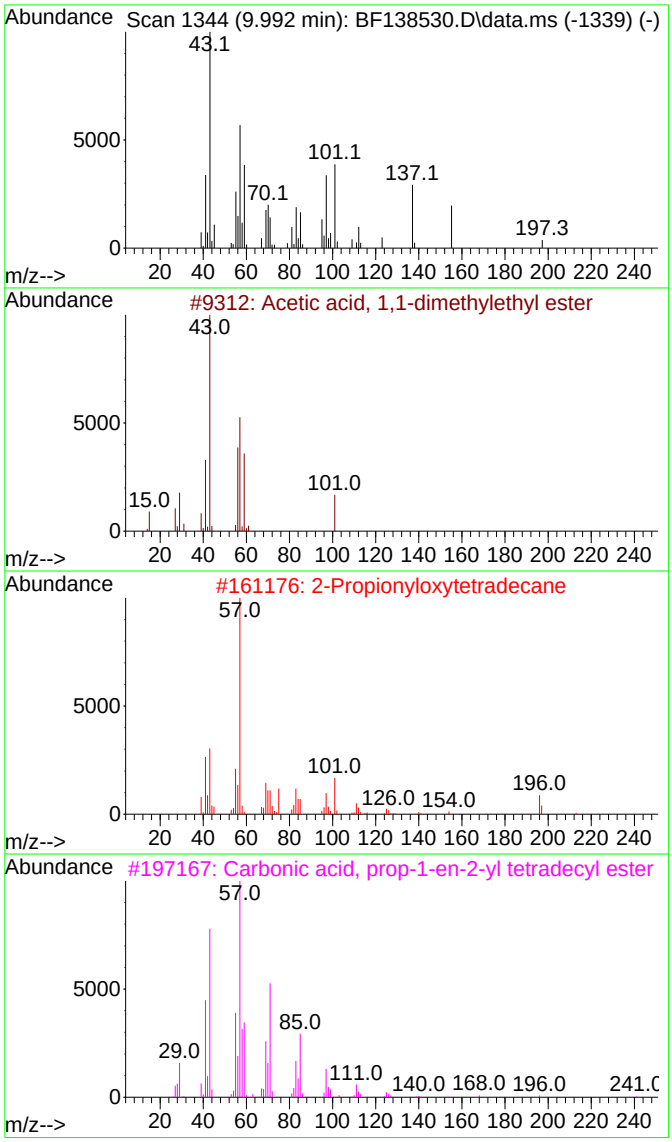
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

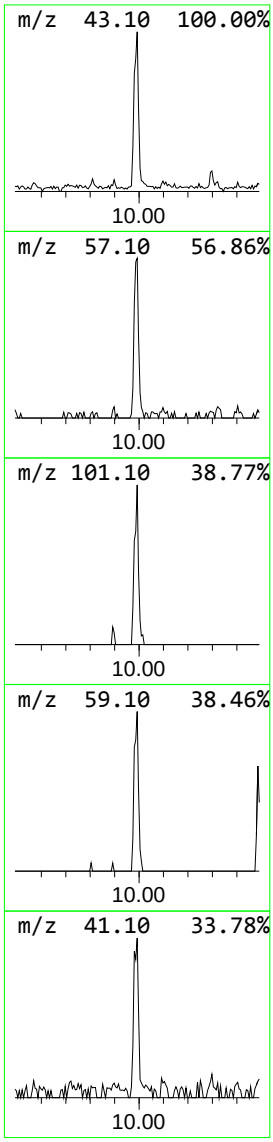
****

Peak Number 3 unknown9.992 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.992	2.08 ng	82091	Acenaphthene-d10	9.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	27
2	2-Propionyloxytetradecane	270	C17H34O2	1000245-62-7	27
3	Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	12
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	11
5	6-Undecen-3-one, 5-butyl-2,2-dim...	252	C17H32O	055976-05-1	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071124\
Data File : BF138530.D
Acq On : 11 Jul 2024 18:48
Operator : CG\JU
Sample : P3187-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

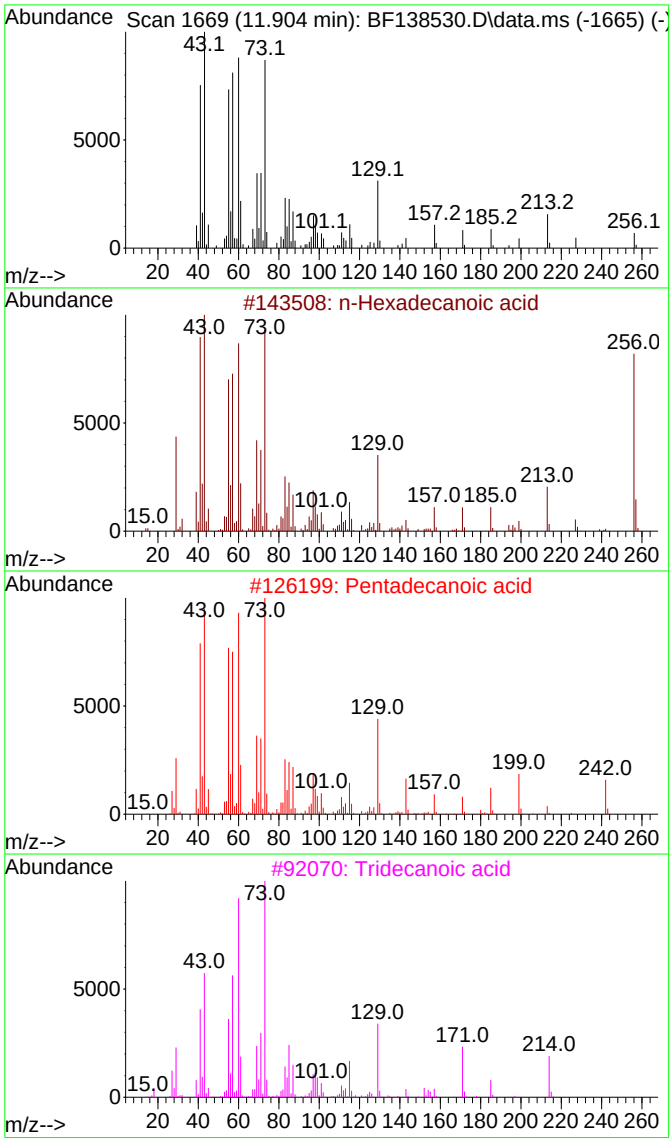
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

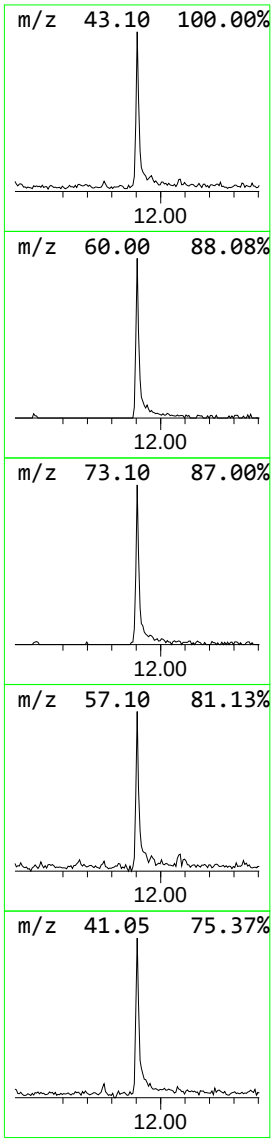
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.904	4.20 ng	144859	Phenanthrene-d10	11.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	86
4	n-Decanoic acid	172	C10H20O2	000334-48-5	86
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071124\
Data File : BF138530.D
Acq On : 11 Jul 2024 18:48
Operator : CG\JU
Sample : P3187-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

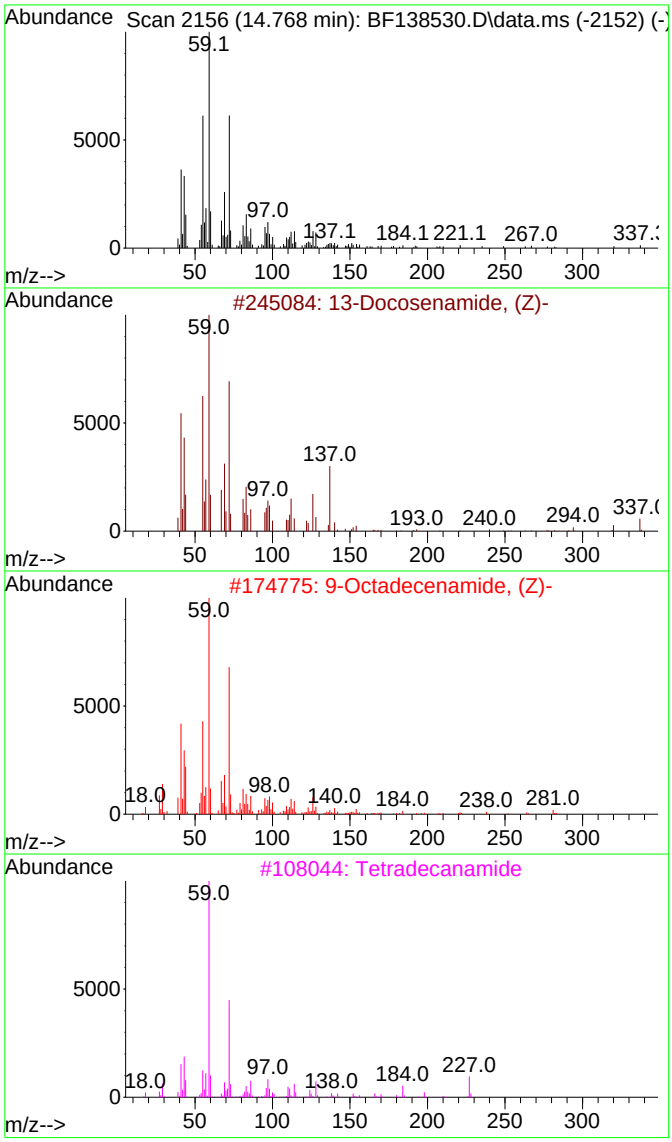
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

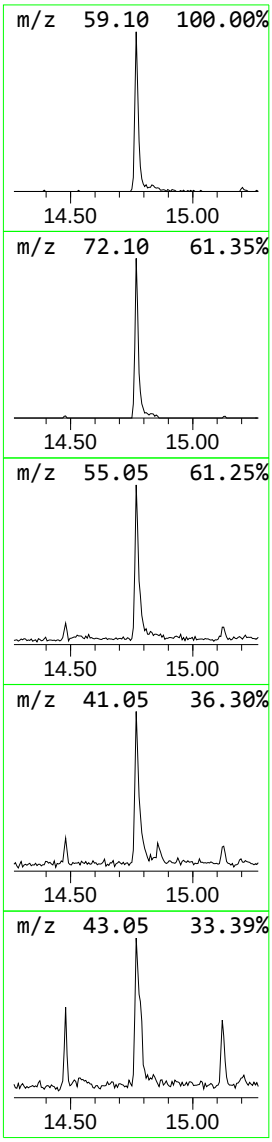
****

Peak Number 5 13-Docosenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.768	9.68 ng	203660	Perylene-d12	15.480

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	Tetradecanamide	227	C14H29NO	000638-58-4	64
4	Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	53
5	Octadecanamide	283	C18H37NO	000124-26-5	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071124\
Data File : BF138530.D
Acq On : 11 Jul 2024 18:48
Operator : CG\JU
Sample : P3187-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.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...	2.169	73.0	ng	2060090	1	6.863	564669	20.0
Propane, 2-meth...	5.086	5.8	ng	163923	1	6.863	564669	20.0
unknown9.992	9.992	2.1	ng	82091	3	9.898	788450	20.0
n-Hexadecanoic ...	11.904	4.2	ng	144859	4	11.380	690104	20.0
13-Docosenamide...	14.768	9.7	ng	203660	6	15.480	420639	20.0