LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110322\
Data File : BF130974.D
Acq On : 03 Nov 2022 23:03
Operator : CG\JU
Sample : N5396-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-I

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: BF130974.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.111	3	4	11	rVB	18505	19137	1.34%	0.172%
2	2.187	11	17	25	rVB	408798	523560	36.58%	4.709%
3	2.299	32	36	44	rVB2	30514	41493	2.90%	0.373%
4	5.134	513	518	527	rBV	313010	333386	23.29%	2.998%
5	5.528	581	585	589	rBV	1368742	1223856	85.50%	11.007%
6	6.534	752	756	759	rBV	1359978	1135303	79.31%	10.210%
7	6.916	818	821	825	rBV	502385	392582	27.43%	3.531%
8	7.481	912	917	920	rBV	812373	718399	50.19%	6.461%
9	8.104	1019	1023	1036	rBV2	94055	232156	16.22%	2.088%
10	8.204	1036	1040	1043	rVB	494530	430662	30.09%	3.873%
11	9.275	1218	1222	1226	rBV	1293615	1159734	81.02%	10.430%
12	9.963	1335	1339	1342	rBV	568057	442806	30.93%	3.982%
13	10.751	1469	1473	1477	rBV	961162	787743	55.03%	7.085%
14	11.457	1589	1593	1596	rBV	635849	538679	37.63%	4.845%
15	11.839	1655	1658	1661	rBV2	66297	55633	3.89%	0.500%
16	11.975	1676	1681	1685	rBV3	17394	29742	2.08%	0.267%
17	12.251	1725	1728	1731	rBV	24207	25658	1.79%	0.231%
18	12.551	1774	1779	1783	rBV5	41254	47790	3.34%	0.430%
19	12.669	1796	1799	1804	rVB	92633	90840	6.35%	0.817%
20	12.904	1833	1839	1842	rBV	100283	124522	8.70%	1.120%
21	13.045	1859	1863	1866	rVB	1729264	1431450	100.00%	12.874%
22	13.298	1904	1906	1909	rBV4	19677	20778	1.45%	0.187%
23	14.104	2039	2043	2046	rBV	674336	602782	42.11%	5.421%
24	14.198	2056	2059	2064	rVB	175489	163944	11.45%	1.474%
25	14.869	2171	2173	2179	rVB2	74570	87191	6.09%	0.784%
26	15.616	2296	2300	2310	rVB	313015	459178	32.08%	4.130%

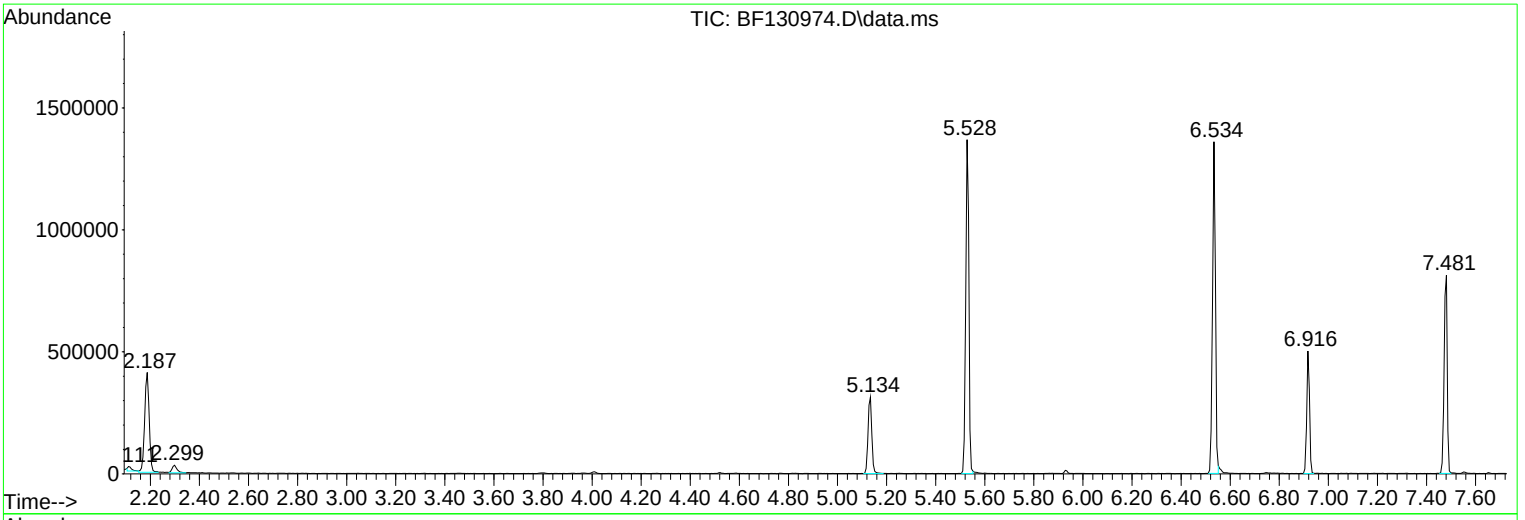
Sum of corrected areas: 11119004

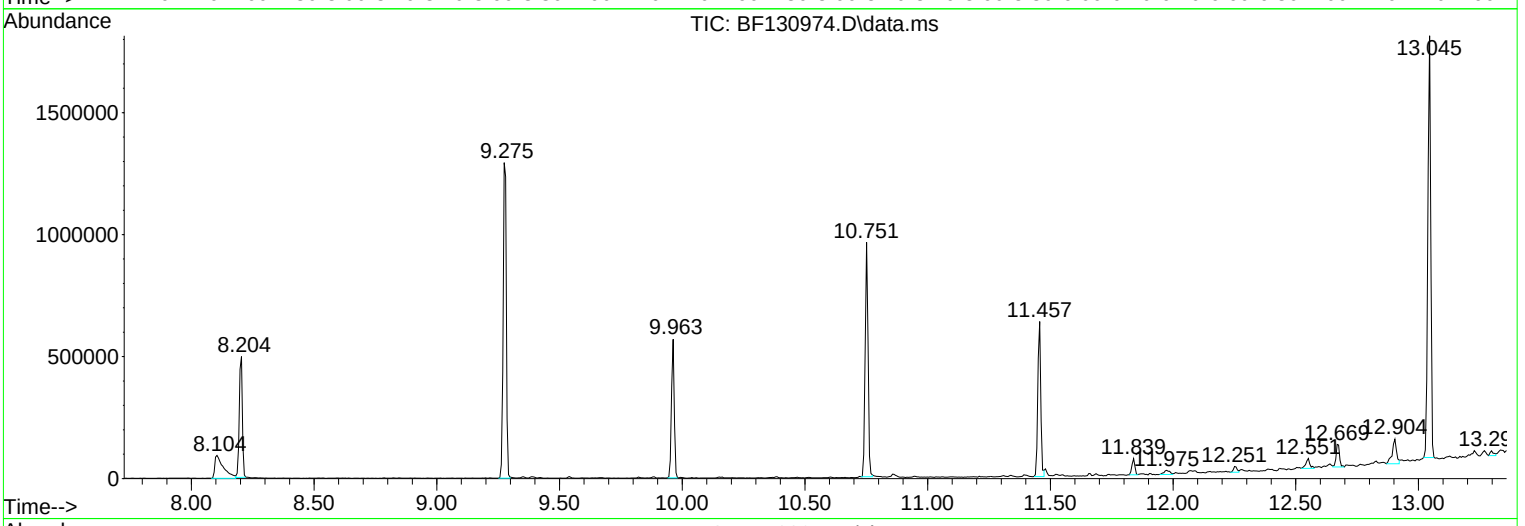
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110322\
Data File : BF130974.D
Acq On : 03 Nov 2022 23:03
Operator : CG\JU
Sample : N5396-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

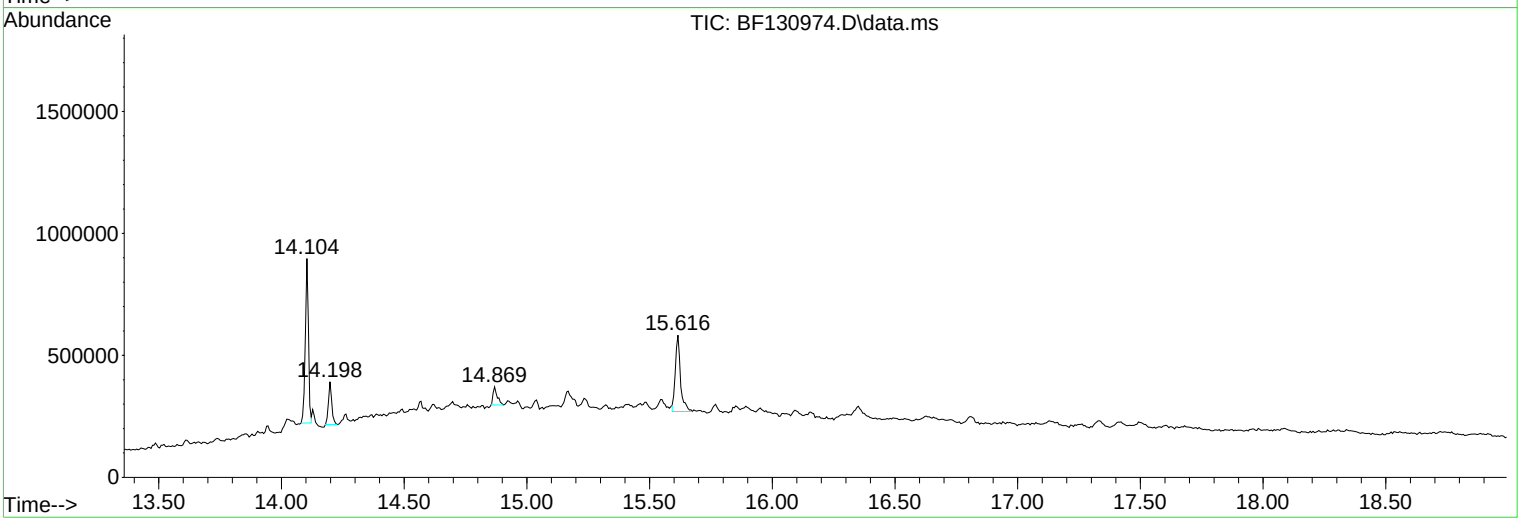
Instrument :
BNA_F
ClientSampleId :
TP-I

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\BF110322\
Data File : BF130974.D
Acq On : 03 Nov 2022 23:03
Operator : CG\JU
Sample : N5396-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-I

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

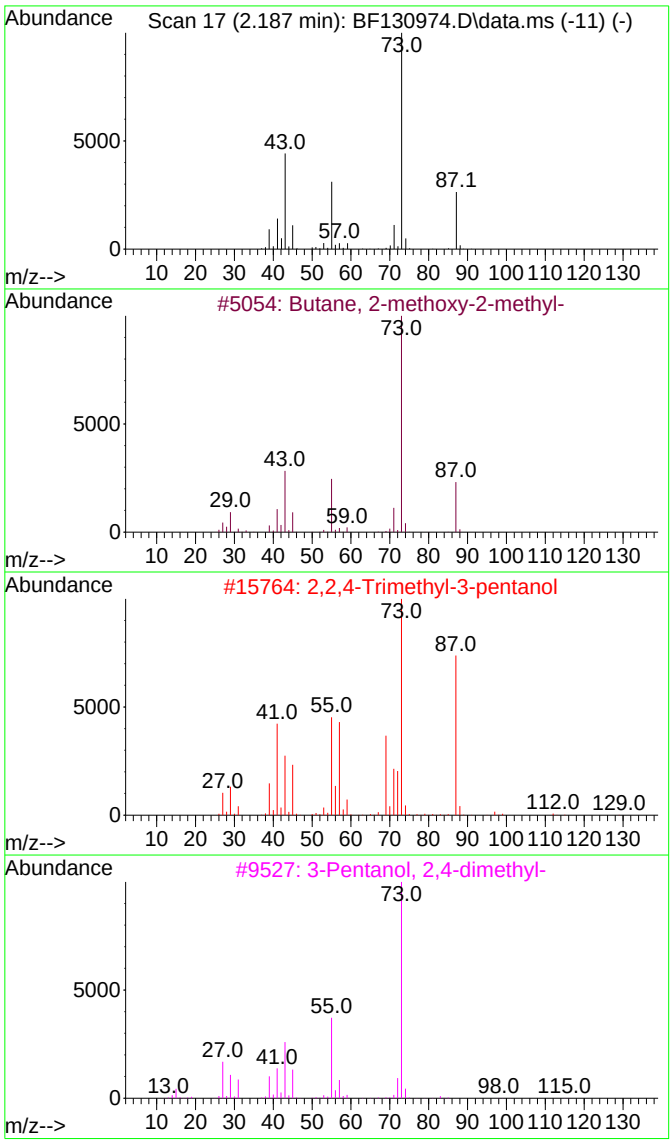
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

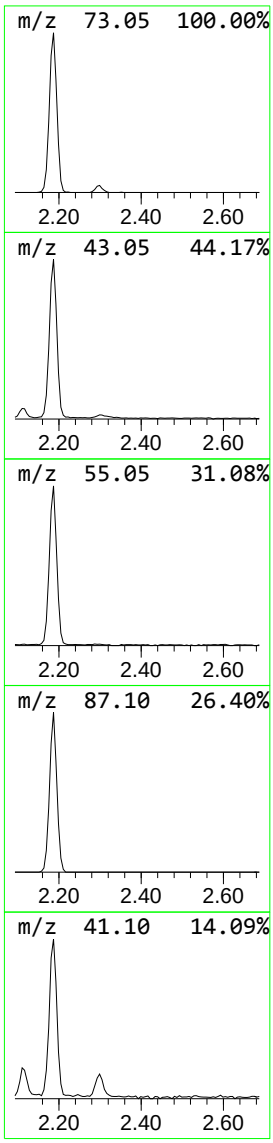
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.187	26.67 ng	523560	1,4-Dichlorobenzene-d4	6.916

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	40
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110322\
Data File : BF130974.D
Acq On : 03 Nov 2022 23:03
Operator : CG\JU
Sample : N5396-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-I

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

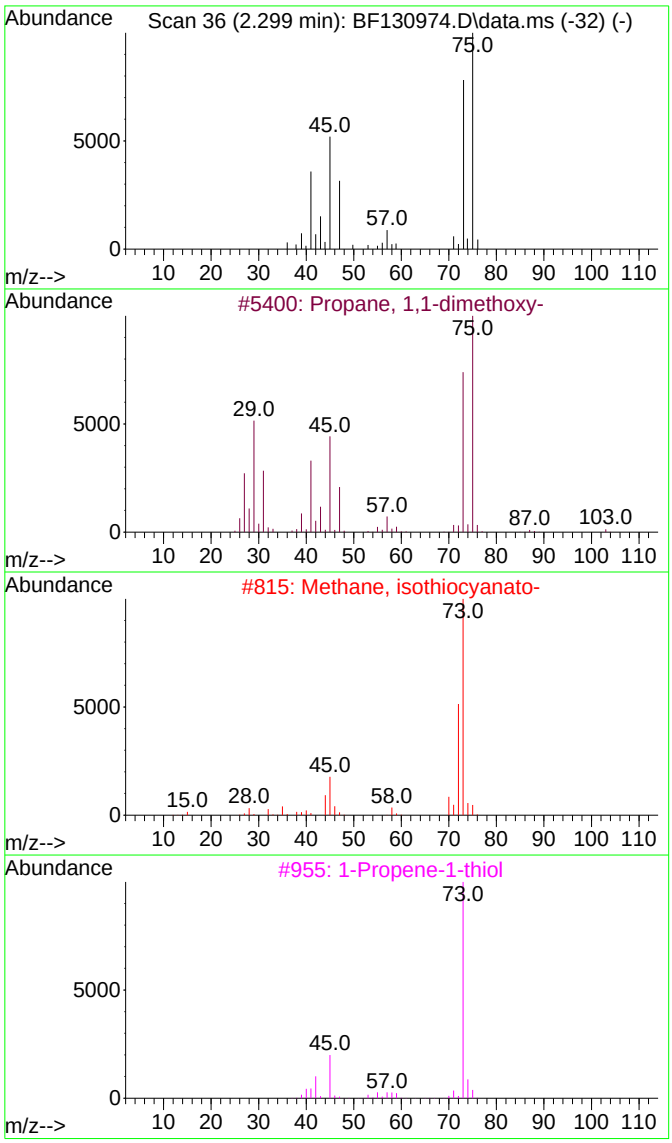
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

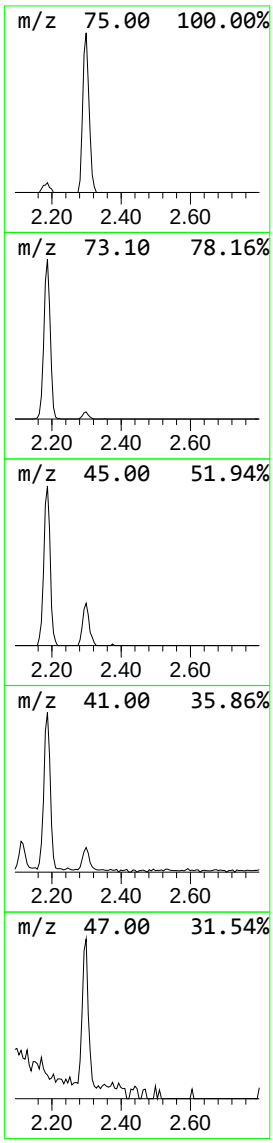
****

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.299	2.11 ng	41493	1,4-Dichlorobenzene-d4	6.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	9
3	1-Propene-1-thiol	74	C3H6S	000925-89-3	9
4	1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	9
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110322\
Data File : BF130974.D
Acq On : 03 Nov 2022 23:03
Operator : CG\JU
Sample : N5396-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-I

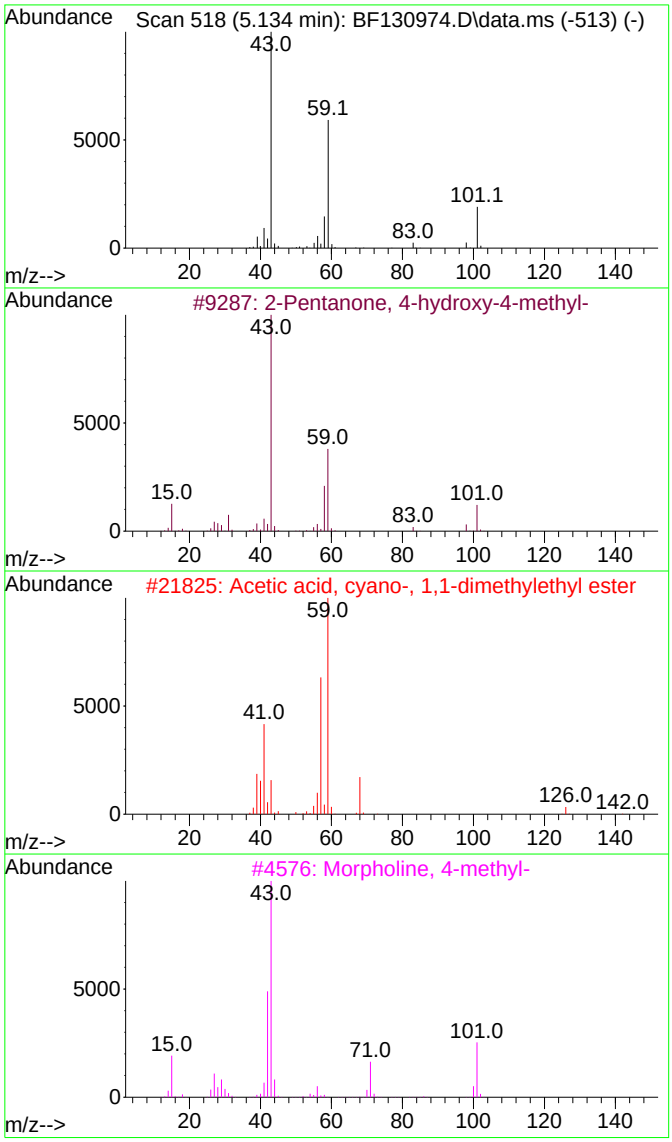
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

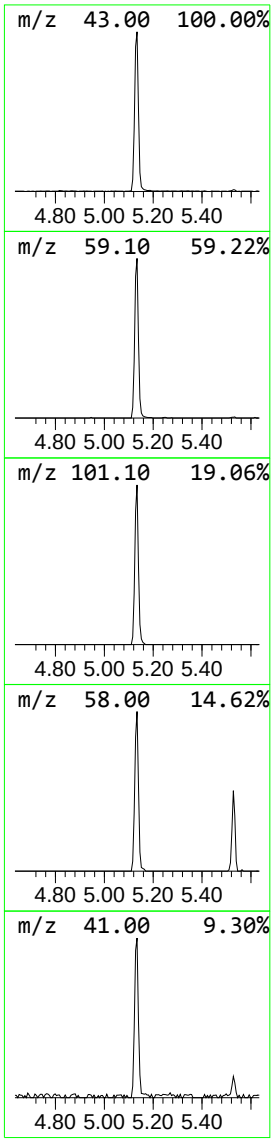
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.134	16.98 ng	333386	1,4-Dichlorobenzene-d4	6.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110322\
Data File : BF130974.D
Acq On : 03 Nov 2022 23:03
Operator : CG\JU
Sample : N5396-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-I

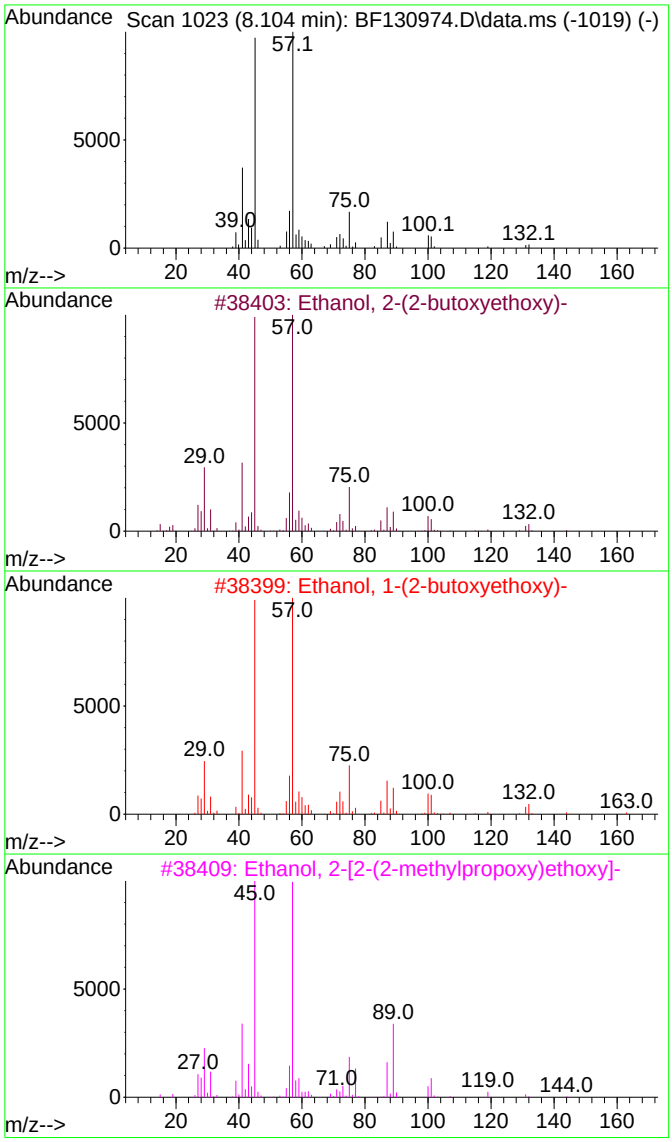
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

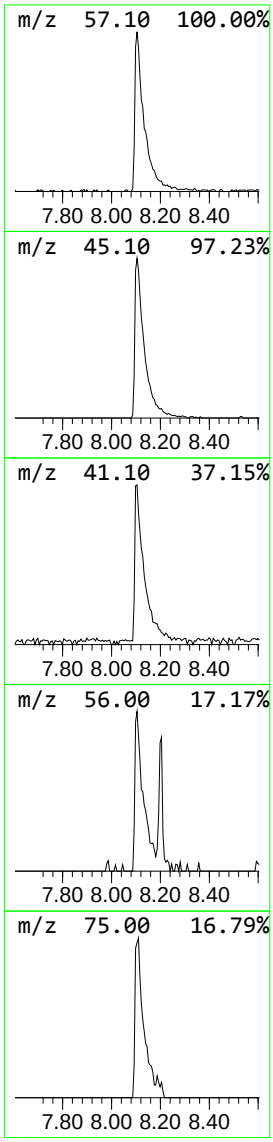
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.104	10.78 ng	232156	Naphthalene-d8	8.204

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
4	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	59
5	Di-sec-Butyl ether	130	C8H18O	006863-58-7	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110322\
Data File : BF130974.D
Acq On : 03 Nov 2022 23:03
Operator : CG\JU
Sample : N5396-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-I

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

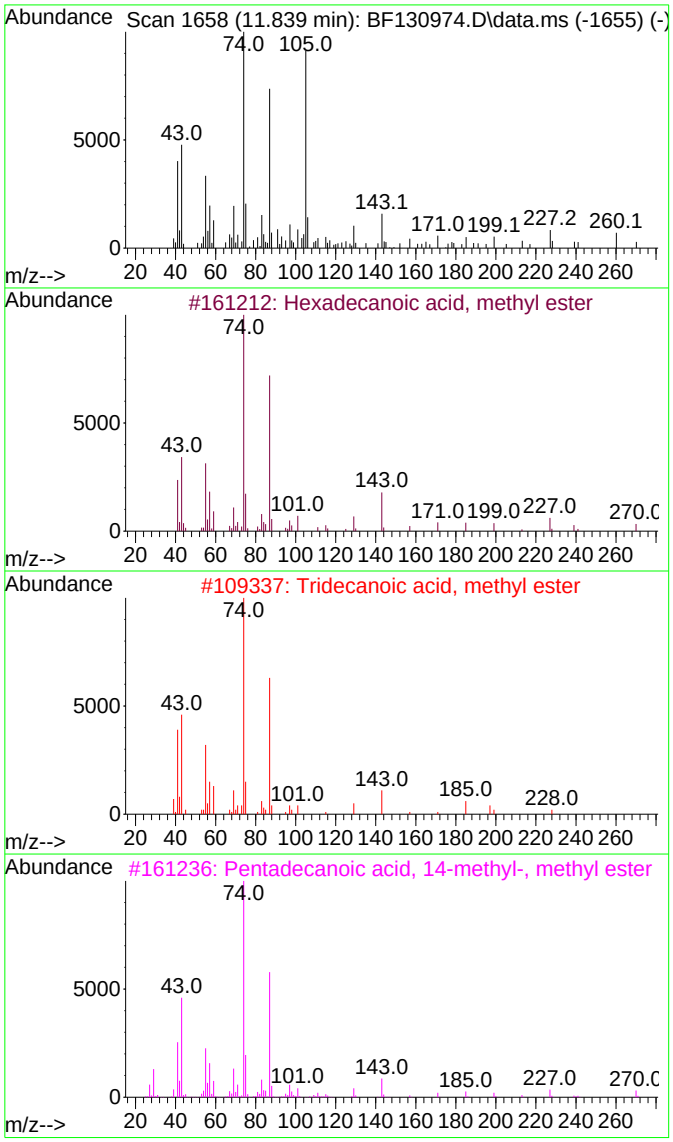
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

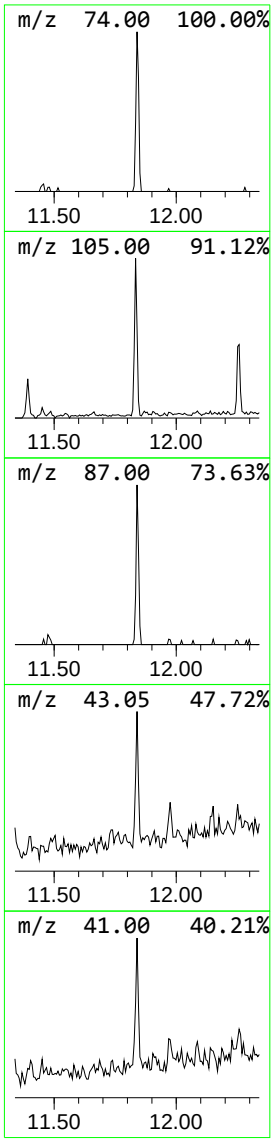
****

Peak Number 5 Hexadecanoic acid, methyl e... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	2.07 ng	55633	Phenanthrene-d10	11.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	97
2	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
3	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	87
4	Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	83
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110322\
Data File : BF130974.D
Acq On : 03 Nov 2022 23:03
Operator : CG\JU
Sample : N5396-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-I

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

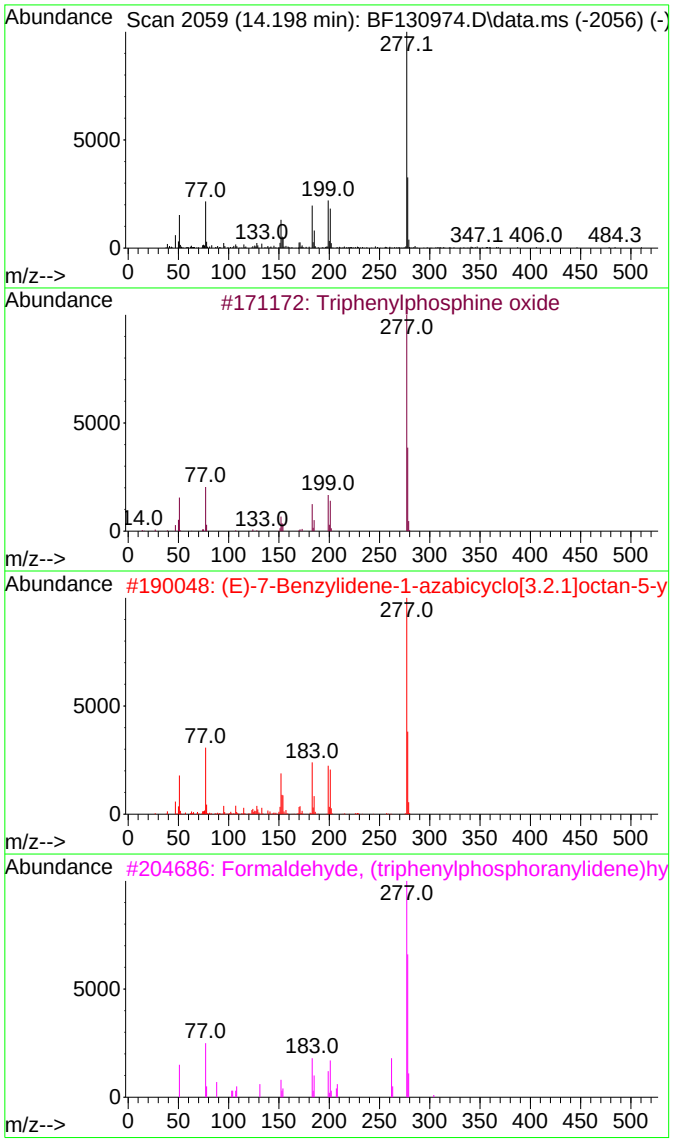
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

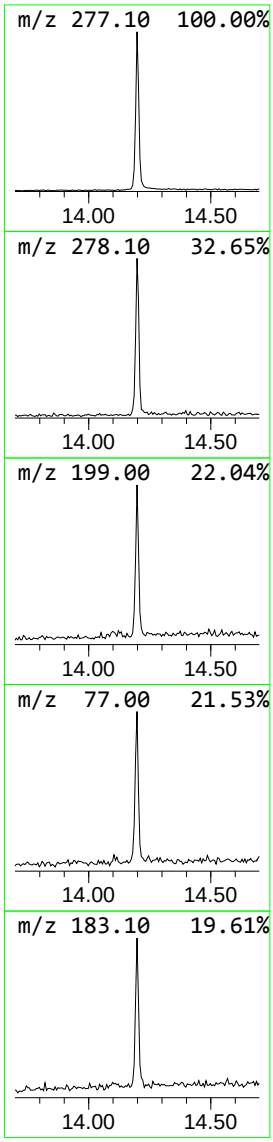
****

Peak Number 6 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.198	5.44 ng	163944	Chrysene-d12	14.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	90
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64
4	(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	50
5	Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	32





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110322\
Data File : BF130974.D
Acq On : 03 Nov 2022 23:03
Operator : CG\JU
Sample : N5396-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-I

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

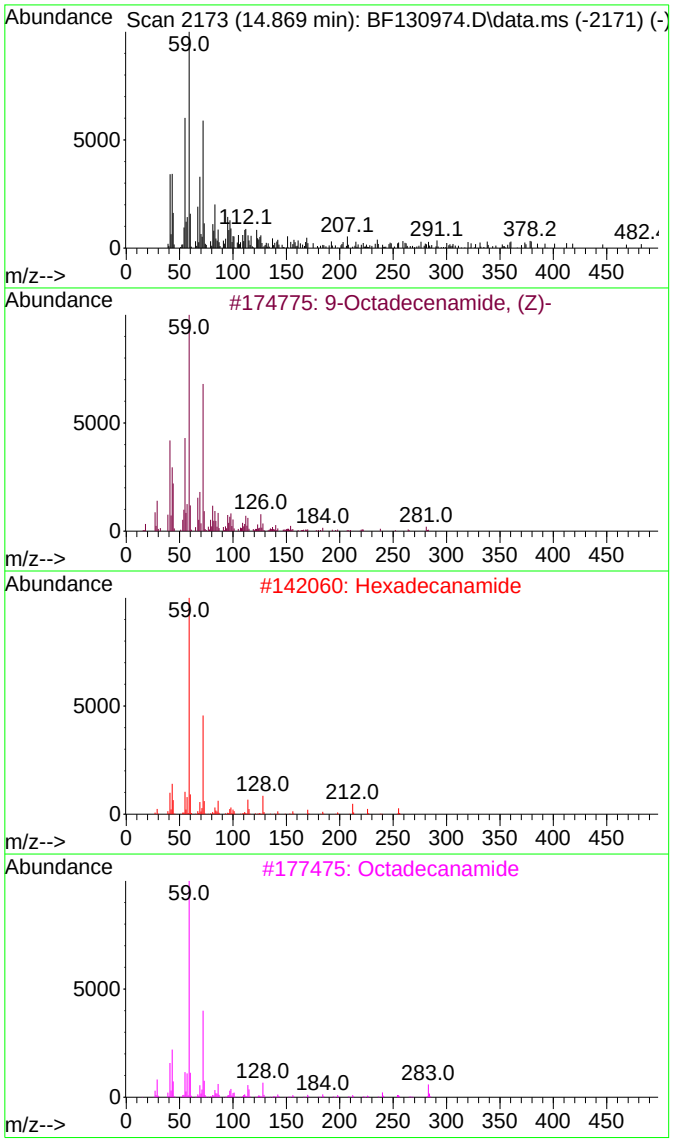
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

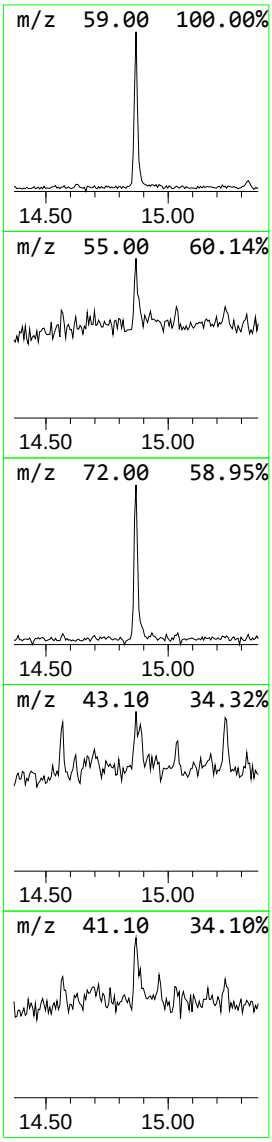
****

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.868	3.80 ng	87191	Perylene-d12	15.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	96
2	Hexadecanamide	255	C16H33NO	000629-54-9	87
3	Octadecanamide	283	C18H37NO	000124-26-5	80
4	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	72
5	Behenic amide	339	C22H45NO	003061-75-4	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110322\
Data File : BF130974.D
Acq On : 03 Nov 2022 23:03
Operator : CG\JU
Sample : N5396-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-I

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...	2.187	26.7	ng	523560	1	6.916	392582	20.0
Propane, 1,1-di...	2.299	2.1	ng	41493	1	6.916	392582	20.0
2-Pentanone, 4-...	5.134	17.0	ng	333386	1	6.916	392582	20.0
Ethanol, 2-(2-b...	8.104	10.8	ng	232156	2	8.204	430662	20.0
Hexadecanoic ac...	11.839	2.1	ng	55633	4	11.457	538679	20.0
Triphenylphosph...	14.198	5.4	ng	163944	5	14.104	602782	20.0
9-Octadecenamid...	14.868	3.8	ng	87191	6	15.616	459178	20.0