LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102822\
Data File : BF130847.D
Acq On : 29 Oct 2022 03:27
Operator : CG\JU
Sample : N5292-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 251032-4

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: BF130847.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.287	27	34	40	rVB	1750230	2343889	62.02%	10.420%
2	5.169	520	524	533	rVB	261248	280404	7.42%	1.247%
3	5.557	585	590	593	rBV	1573598	1378597	36.48%	6.129%
4	6.551	754	759	762	rBV	996683	851337	22.53%	3.785%
5	6.945	822	826	829	rVB	777790	628327	16.63%	2.793%
6	7.510	916	922	925	rBV	2099659	2131473	56.40%	9.476%
7	8.128	1022	1027	1039	rBV	591482	639334	16.92%	2.842%
8	8.228	1039	1044	1048	rVB	915800	807221	21.36%	3.589%
9	9.310	1222	1228	1231	rBV	3768766	3778990	100.00%	16.800%
10	9.416	1242	1246	1254	rVB	332387	287474	7.61%	1.278%
11	9.698	1289	1294	1297	rBV	92313	67885	1.80%	0.302%
12	9.986	1338	1343	1347	rBV	1015977	918588	24.31%	4.084%
13	10.780	1471	1478	1481	rBV	2629782	2306665	61.04%	10.254%
14	11.480	1593	1597	1600	rBV	1123785	914028	24.19%	4.063%
15	11.869	1659	1663	1666	rVB	146465	112206	2.97%	0.499%
16	12.574	1777	1783	1792	rVB	292327	280560	7.42%	1.247%
17	12.663	1792	1798	1801	rBV	81628	70183	1.86%	0.312%
18	13.074	1863	1868	1871	rBV	3391411	3100284	82.04%	13.782%
19	14.016	2022	2028	2038	rBV9	13817	39368	1.04%	0.175%
20	14.121	2043	2046	2050	rVB	704661	662481	17.53%	2.945%
21	14.221	2057	2063	2070	rBV	222760	243892	6.45%	1.084%
22	14.998	2191	2195	2199	rBV	156613	161546	4.27%	0.718%
23	15.639	2299	2304	2309	rBV	397591	489681	12.96%	2.177%

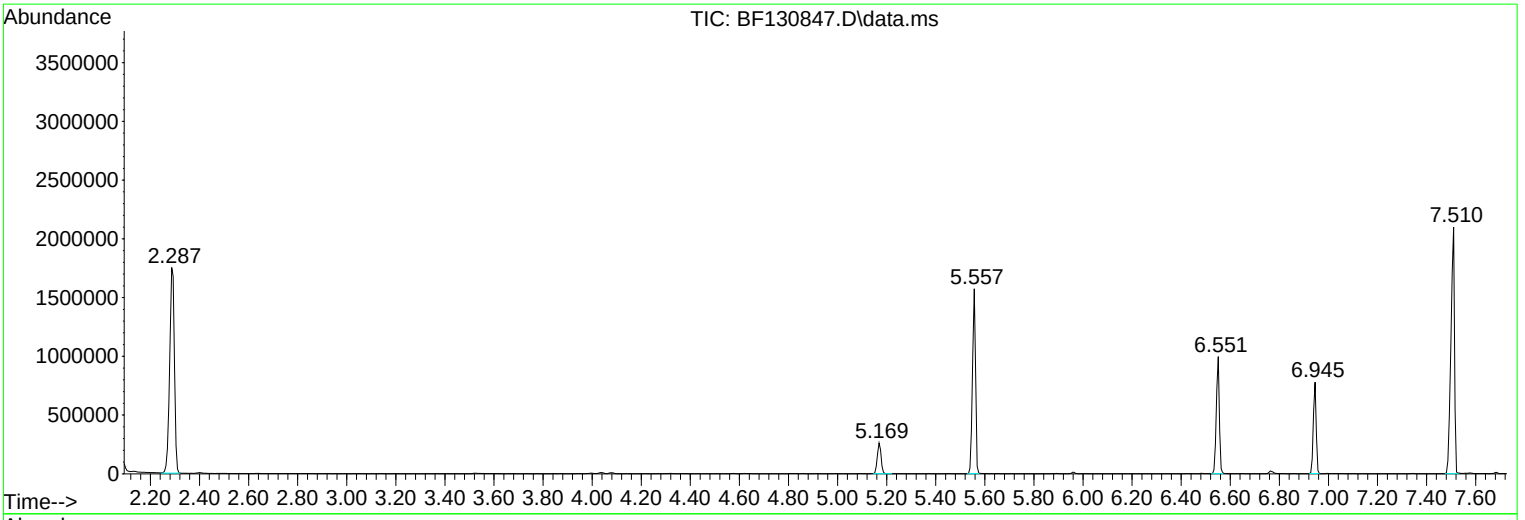
Sum of corrected areas: 22494413

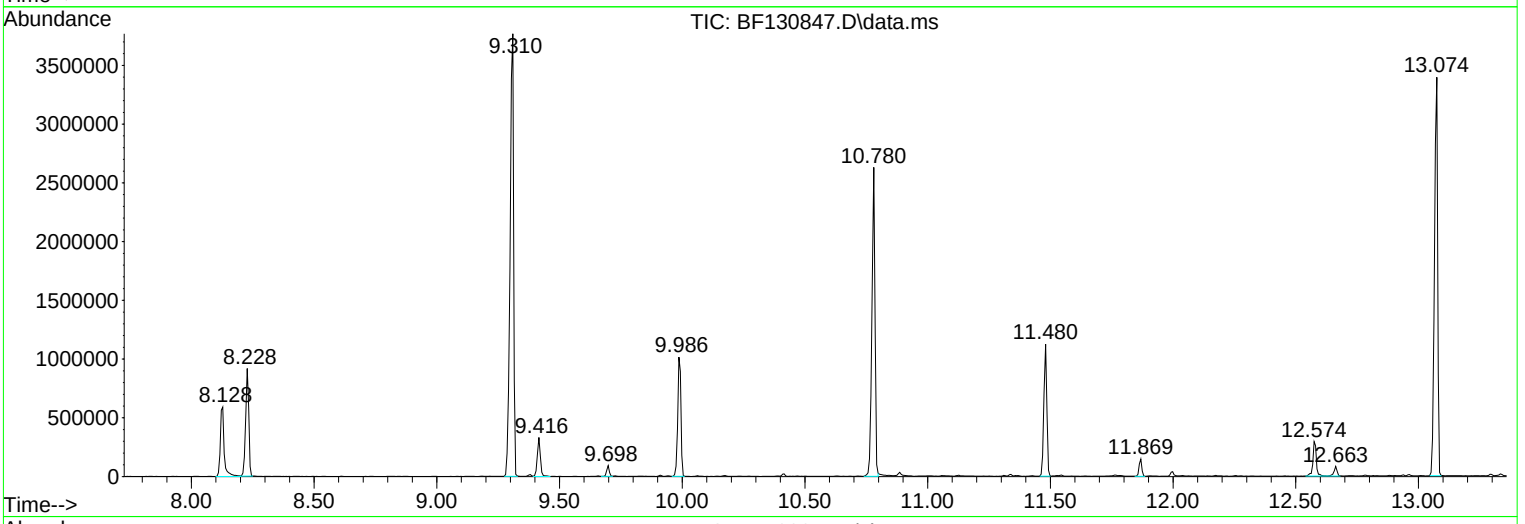
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102822\
Data File : BF130847.D
Acq On : 29 Oct 2022 03:27
Operator : CG\JU
Sample : N5292-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

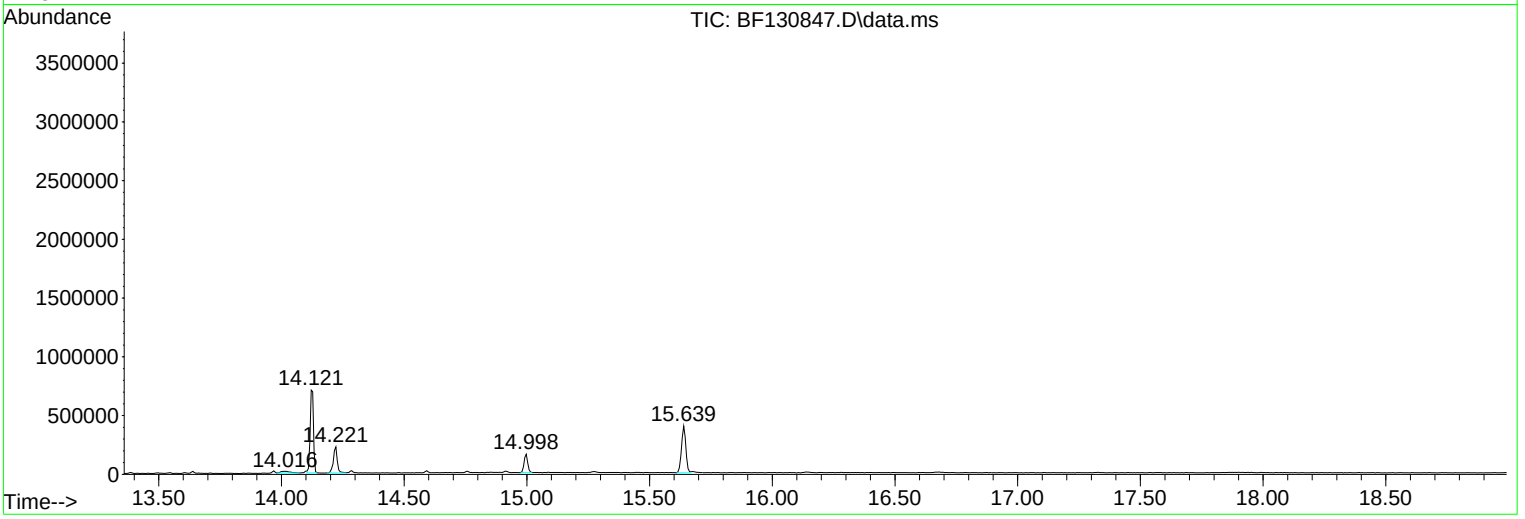
Instrument :
BNA_F
ClientSampleId :
251032-4

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







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Data File : BF130847.D
Acq On : 29 Oct 2022 03:27
Operator : CG\JU
Sample : N5292-02
Misc :
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

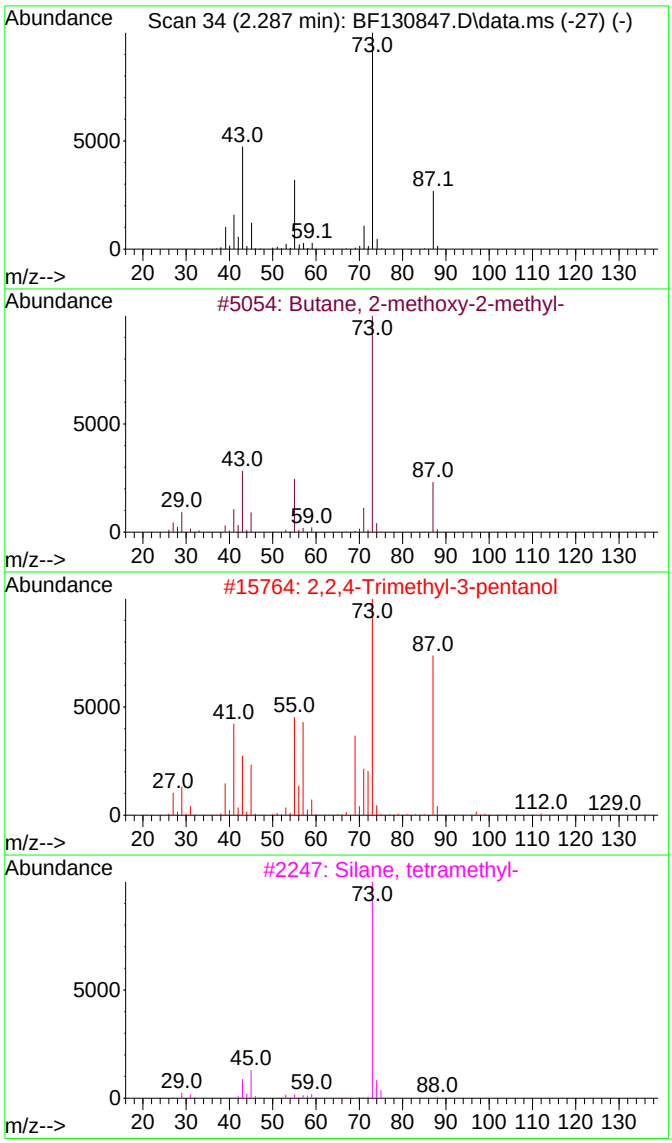
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

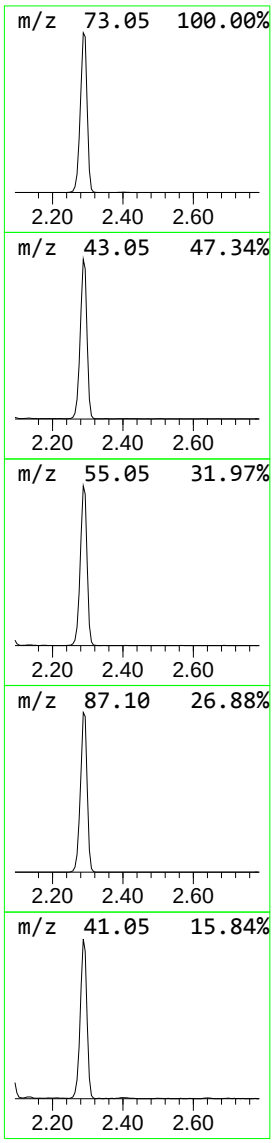
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.287	74.61 ng	2343890	1,4-Dichlorobenzene-d4	6.945

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	38
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9





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Data File : BF130847.D
Acq On : 29 Oct 2022 03:27
Operator : CG\JU
Sample : N5292-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
251032-4

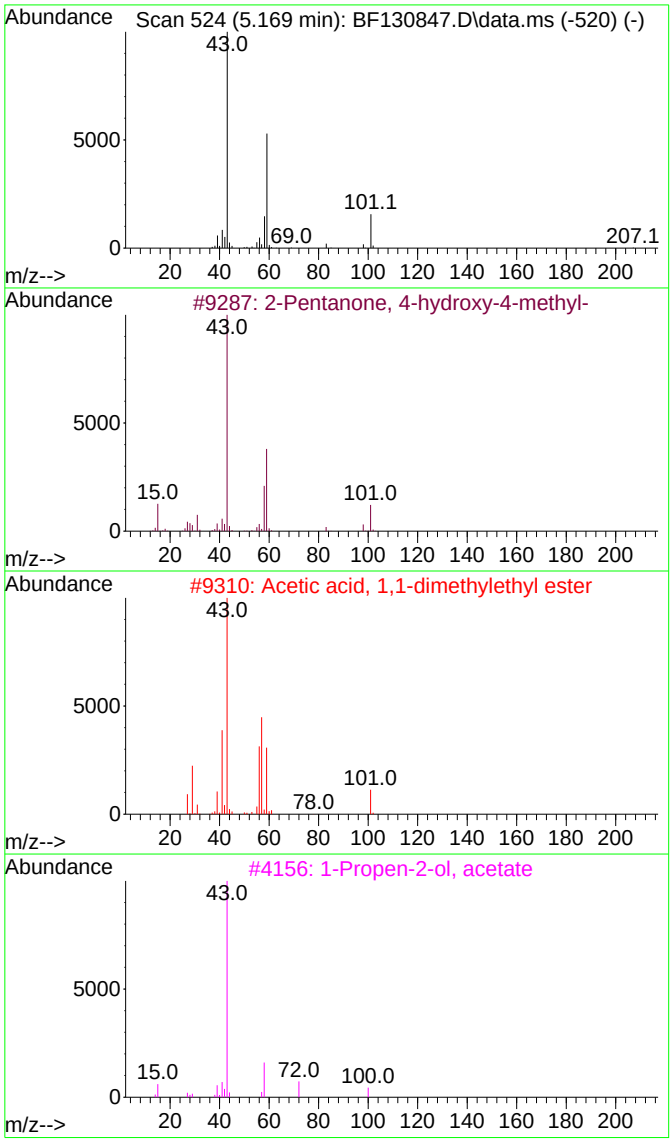
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

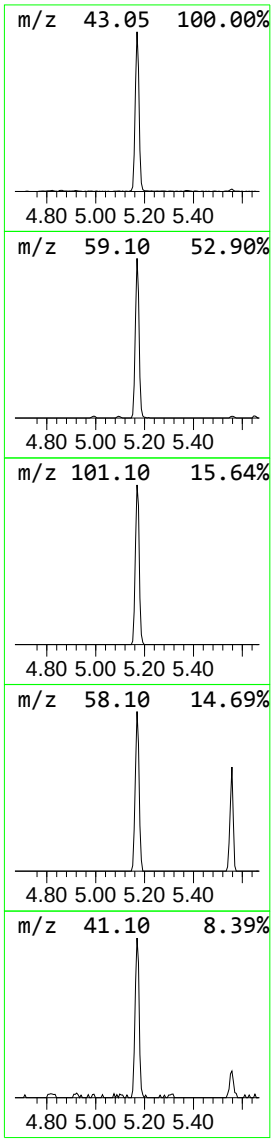
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.169	8.93 ng	280404	1,4-Dichlorobenzene-d4	6.945

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9





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Acq On : 29 Oct 2022 03:27
Operator : CG\JU
Sample : N5292-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
251032-4

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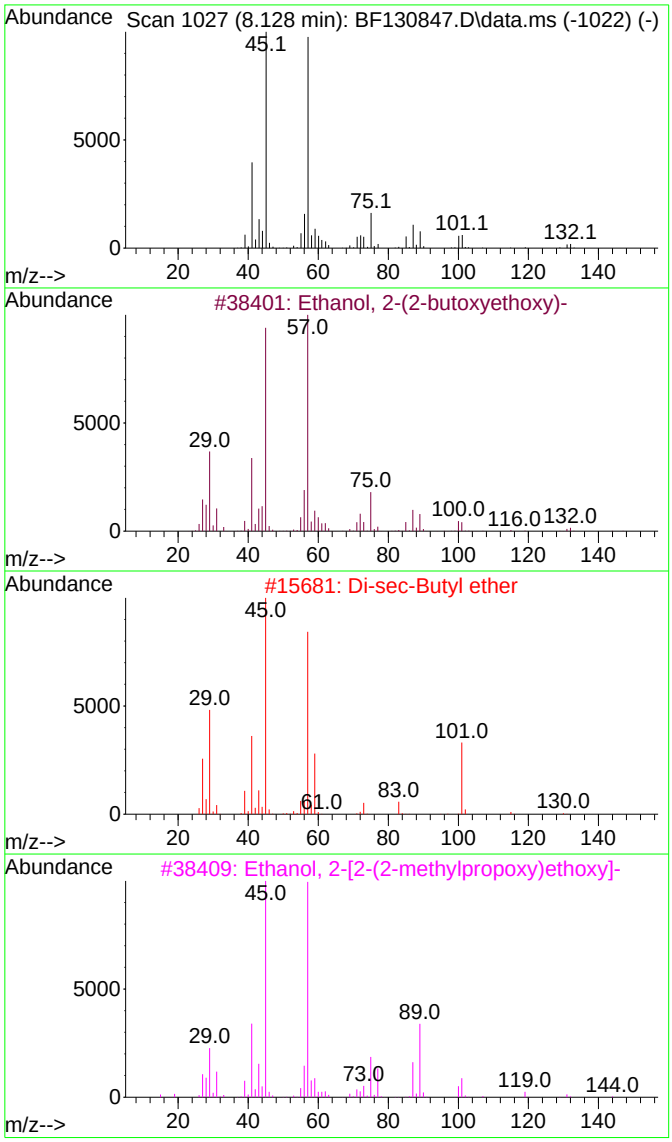
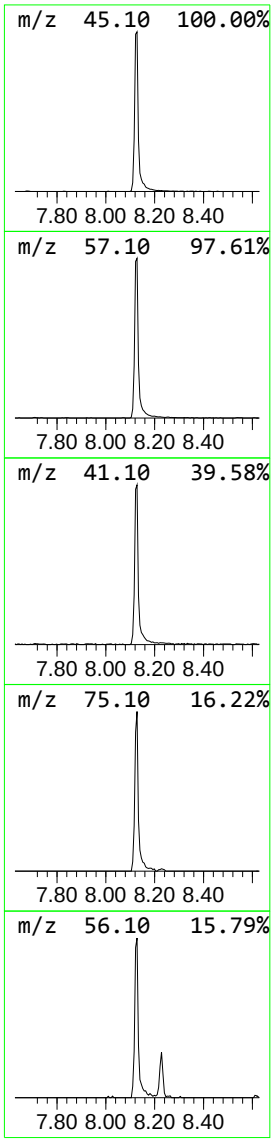
****
Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.128	15.84 ng	639334	Naphthalene-d8	8.228

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Di-sec-Butyl ether	130	C8H18O	006863-58-7	59
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50
5	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50





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Acq On : 29 Oct 2022 03:27
Operator : CG\JU
Sample : N5292-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
251032-4

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

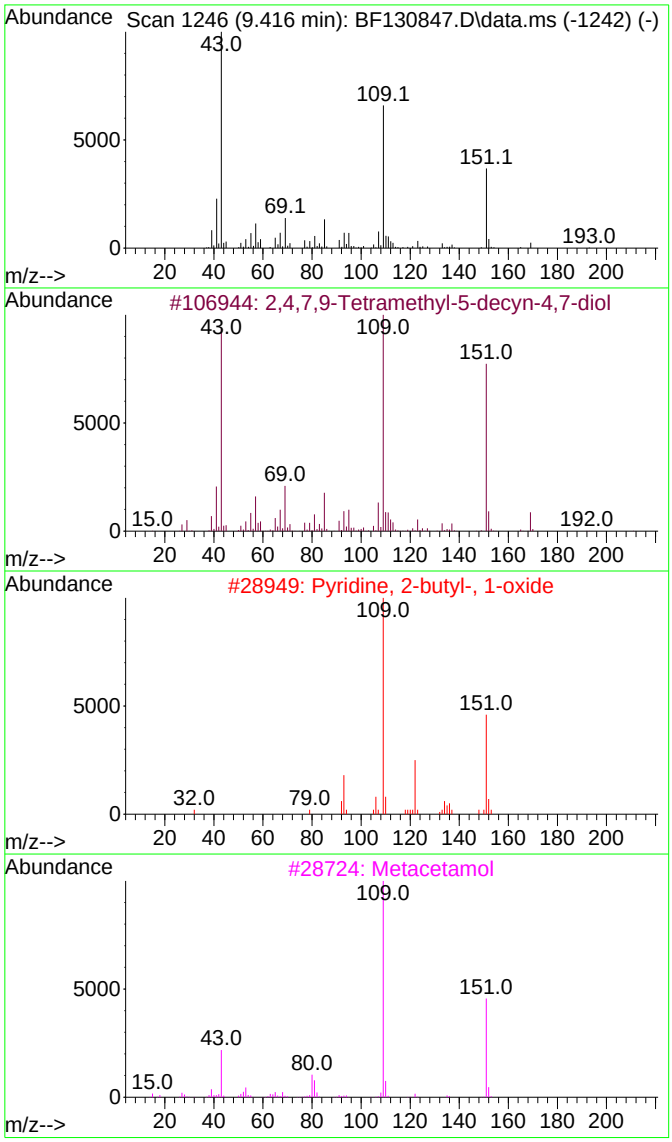
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

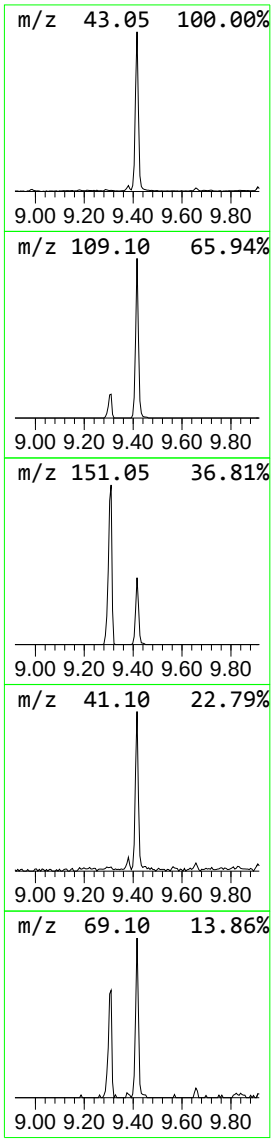
****

Peak Number 4 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.416	6.26 ng	287474	Acenaphthene-d10	9.986

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	87
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	53
3	Metacetamol	151	C8H9NO2	000621-42-1	49
4	Acetaminophen	151	C8H9NO2	000103-90-2	47
5	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	47





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Acq On : 29 Oct 2022 03:27
Operator : CG\JU
Sample : N5292-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
251032-4

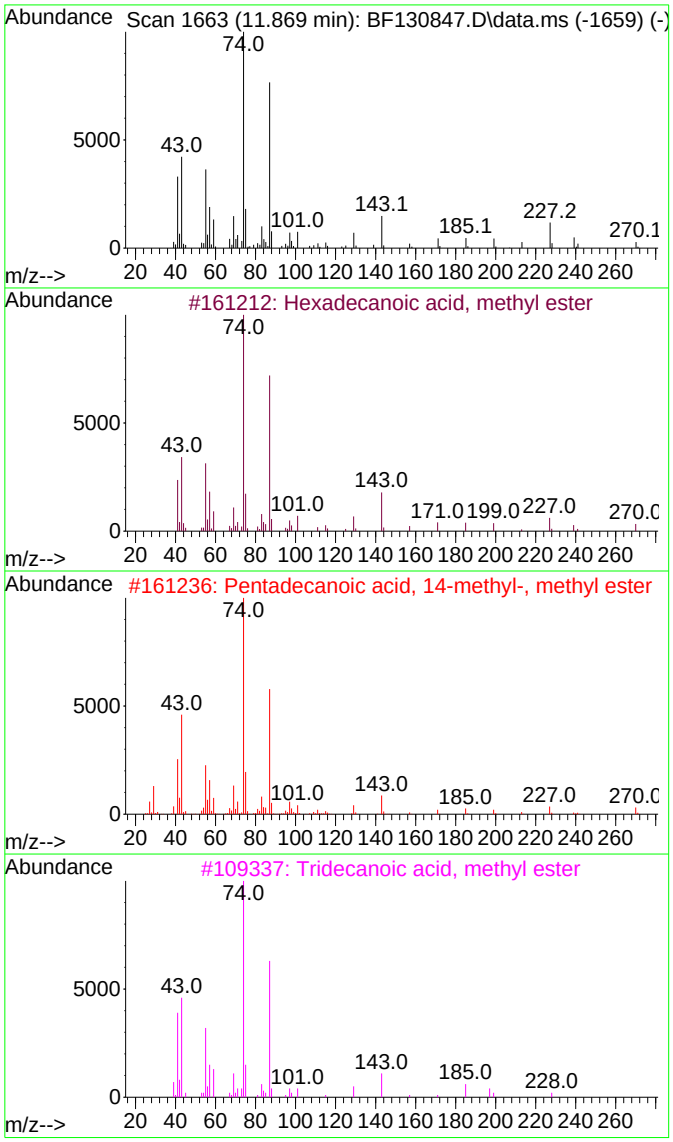
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

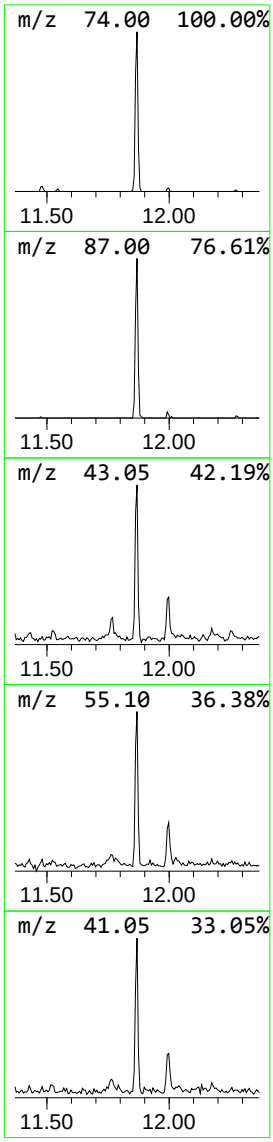
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Hexadecanoic acid, methyl e... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.869	2.46 ng	112206	Phenanthrene-d10	11.480

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	96
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	93
4	Methyl 8-methyl-nonanoate	186	C11H22O2	1000452-00-9	90
5	Dodecanoic acid, 10-methyl-, met...	228	C14H28O2	005129-65-7	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102822\
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Operator : CG\JU
Sample : N5292-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
251032-4

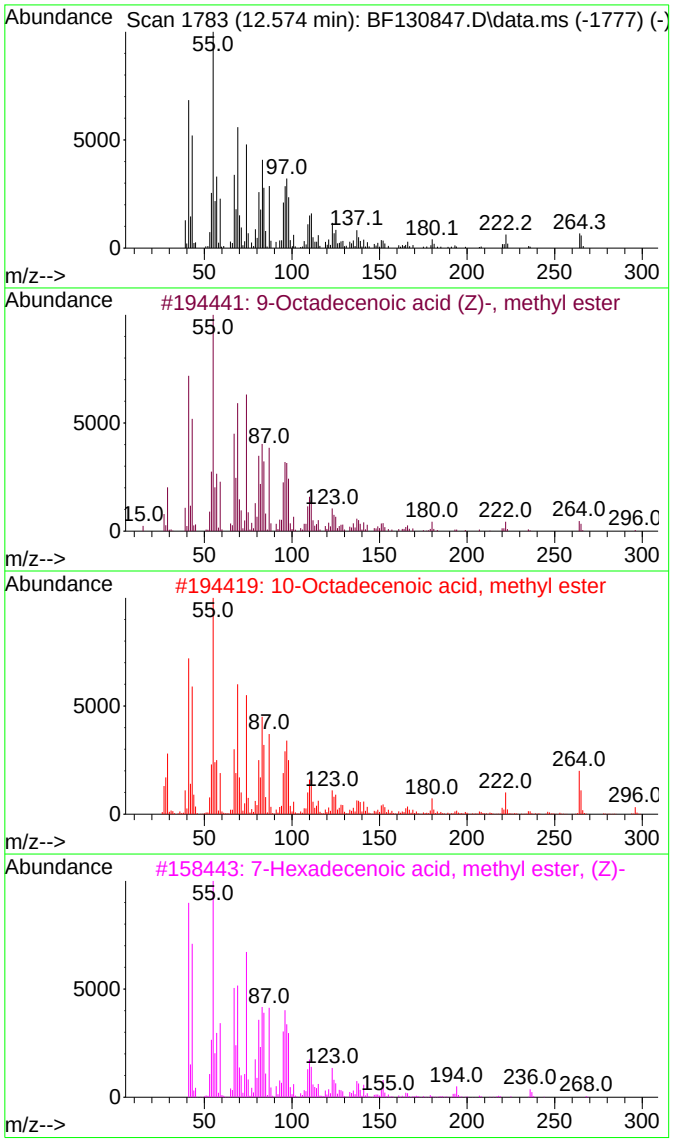
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

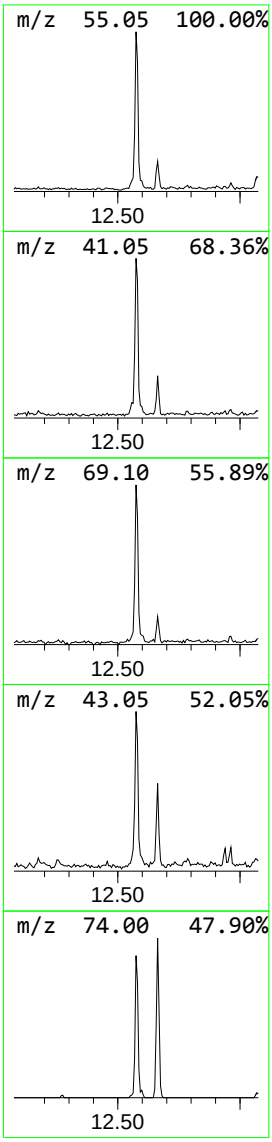
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 9-Octadecenoic acid (Z)-, m... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.574	6.14 ng	280560	Phenanthrene-d10	11.480

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	95
2	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	94
3	7-Hexadecenoic acid, methyl este...	268	C17H32O2	056875-67-3	91
4	9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	87
5	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	86





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Sample : N5292-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
251032-4

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

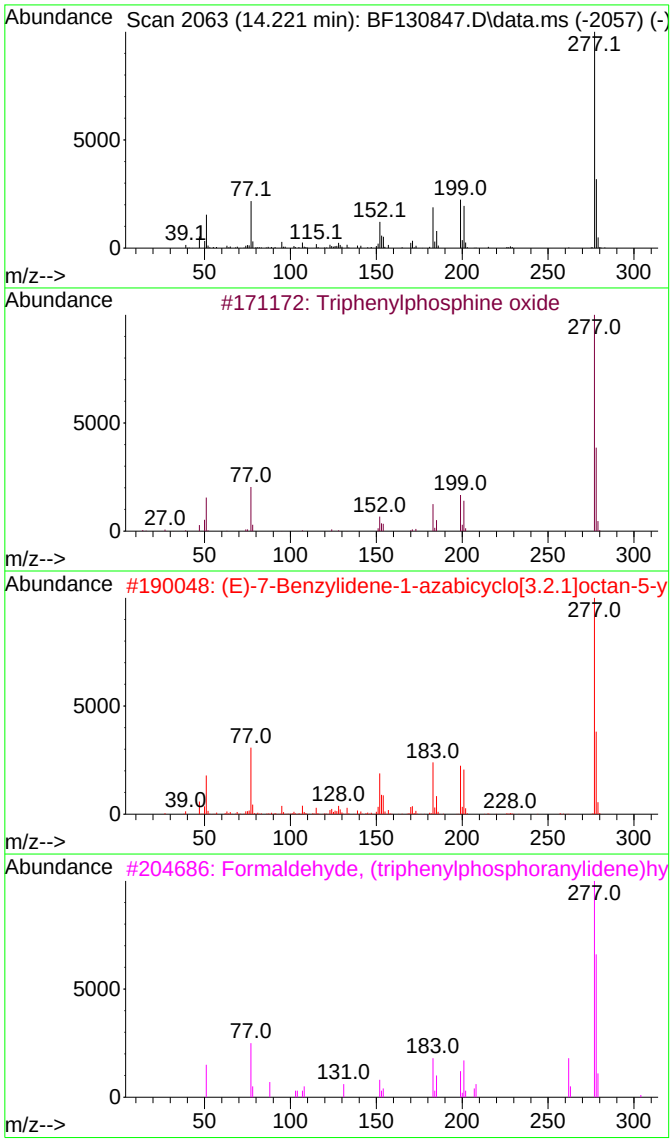
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

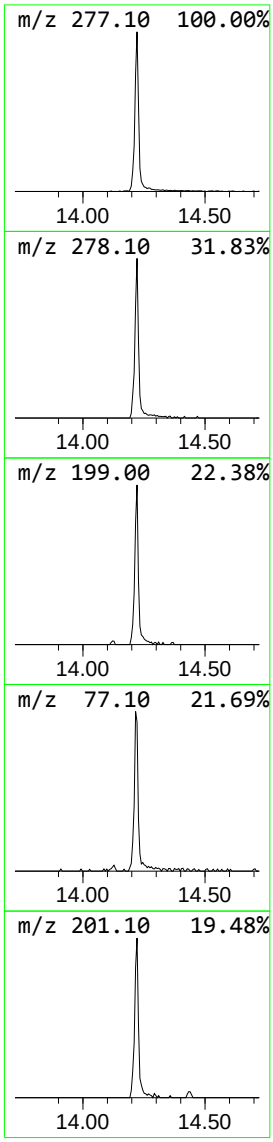
****

Peak Number 7 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.221	7.36 ng	243892	Chrysene-d12	14.127

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	87
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
4	3-(3,4-Dichlorophenyl)-2-thioxo-...	277	C9H5Cl2NOS2	017046-34-3	38
5	1H-Indole-3-acetic acid, 5-[(tri...	277	C14H19NO3Si	072101-35-0	23





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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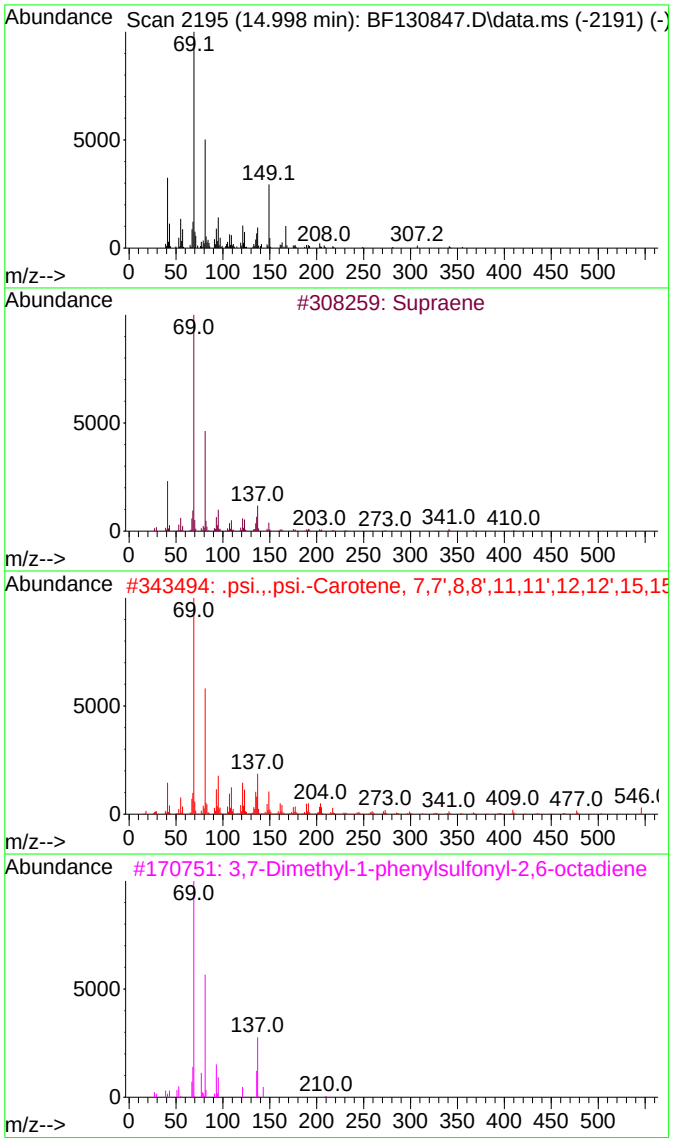
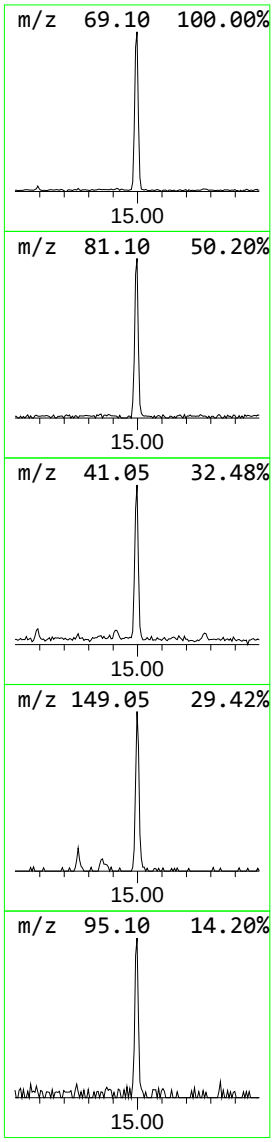
****

Peak Number 8 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.998	6.60 ng	161546	Perylene-d12	15.639

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	62
2	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	59
3	3,7-Dimethyl-1-phenylsulfonyl-2,...	278	C16H22O2S	1000432-27-5	53
4	Trifluoroacetyl-lavandulol	250	C12H17F3O2	028673-24-7	53
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	53





Tentatively Identified Compound (LSC) summary

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Data File : BF130847.D
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ClientSampleId :
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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...	2.287	74.6	ng	2343890	1	6.945	628327	20.0
2-Pentanone, 4-...	5.169	8.9	ng	280404	1	6.945	628327	20.0
Ethanol, 2-(2-b...	8.128	15.8	ng	639334	2	8.228	807221	20.0
2,4,7,9-Tetrame...	9.416	6.3	ng	287474	3	9.986	918588	20.0
Hexadecanoic ac...	11.869	2.5	ng	112206	4	11.480	914028	20.0
9-Octadecenoic ...	12.574	6.1	ng	280560	4	11.480	914028	20.0
Triphenylphosph...	14.221	7.4	ng	243892	5	14.127	662481	20.0
Supraene	14.998	6.6	ng	161546	6	15.639	489681	20.0