LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102822\
Data File : BF130831.D
Acq On : 28 Oct 2022 19:25
Operator : CG\JU
Sample : N5281-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-12

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: BF130831.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.293	25	35	41	rVB	1145150	1532478	57.43%	7.836%
2	3.510	239	242	251	rBV	17398	32668	1.22%	0.167%
3	5.181	521	526	533	rVB	284714	340472	12.76%	1.741%
4	5.563	586	591	594	rBV	2376878	2218161	83.12%	11.342%
5	6.557	755	760	763	rBV	2147469	2281144	85.49%	11.664%
6	6.945	822	826	829	rBV	797420	613579	22.99%	3.137%
7	7.504	916	921	924	rBV	1422953	1403662	52.60%	7.177%
8	8.228	1040	1044	1048	rBV	919573	796217	29.84%	4.071%
9	9.310	1222	1228	1231	rBV	2655800	2668465	100.00%	13.644%
10	9.992	1338	1344	1347	rVB	976436	906440	33.97%	4.635%
11	10.780	1473	1478	1481	rBV	1648939	1588461	59.53%	8.122%
12	11.480	1593	1597	1600	rBV	1136875	896794	33.61%	4.585%
13	11.545	1605	1608	1611	rVB2	42506	31027	1.16%	0.159%
14	11.998	1678	1685	1690	rBV	56492	68194	2.56%	0.349%
15	12.827	1820	1826	1829	rVB	99735	116291	4.36%	0.595%
16	12.910	1835	1840	1846	rVB	111699	117194	4.39%	0.599%
17	13.068	1863	1867	1871	rBV	2513025	2367993	88.74%	12.108%
18	13.980	2016	2022	2030	rBV2	75854	148432	5.56%	0.759%
19	14.127	2043	2047	2050	rVB	711350	648319	24.30%	3.315%
20	14.221	2058	2063	2067	rBV	102092	116210	4.35%	0.594%
21	14.557	2113	2120	2124	rBV5	31401	52988	1.99%	0.271%
22	14.898	2174	2178	2184	rVB4	51100	73479	2.75%	0.376%
23	14.998	2192	2195	2200	rVB	27500	29817	1.12%	0.152%
24	15.639	2299	2304	2314	rVB	408374	508761	19.07%	2.601%

Sum of corrected areas: 19557246

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Instrument :
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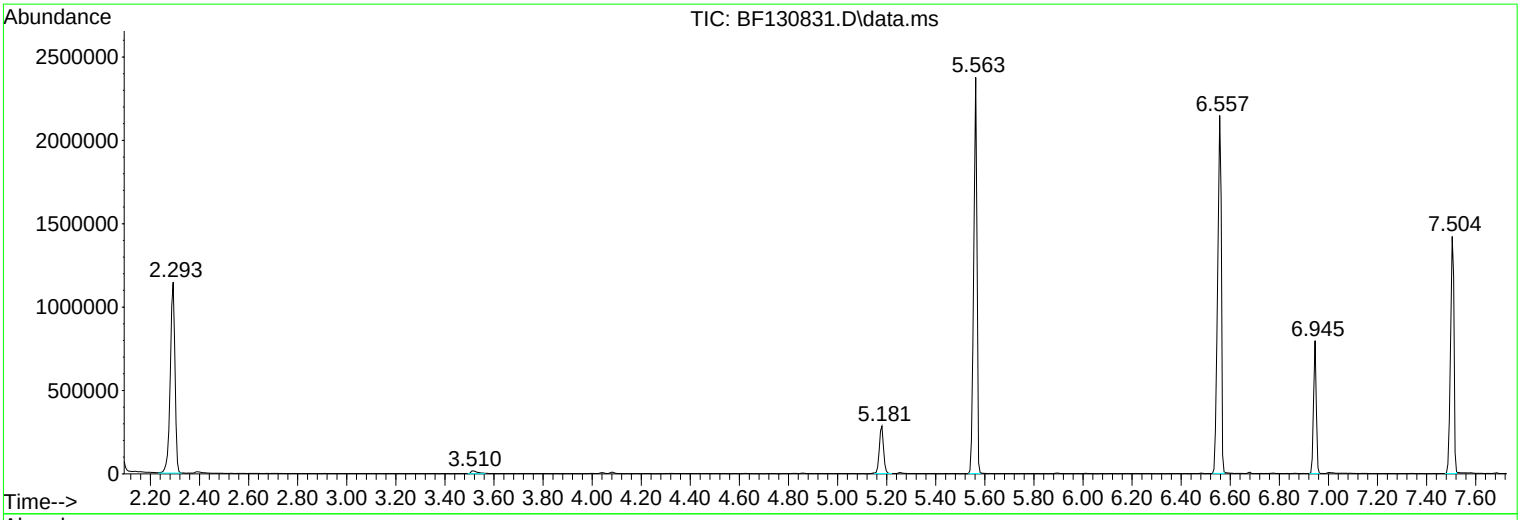
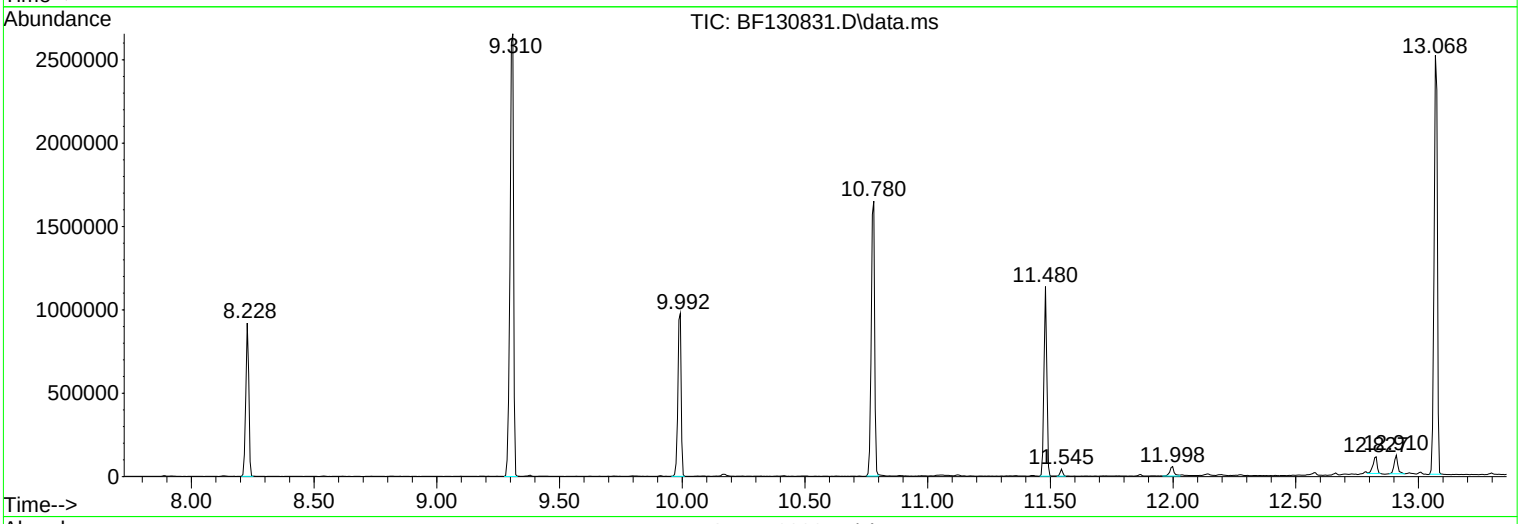
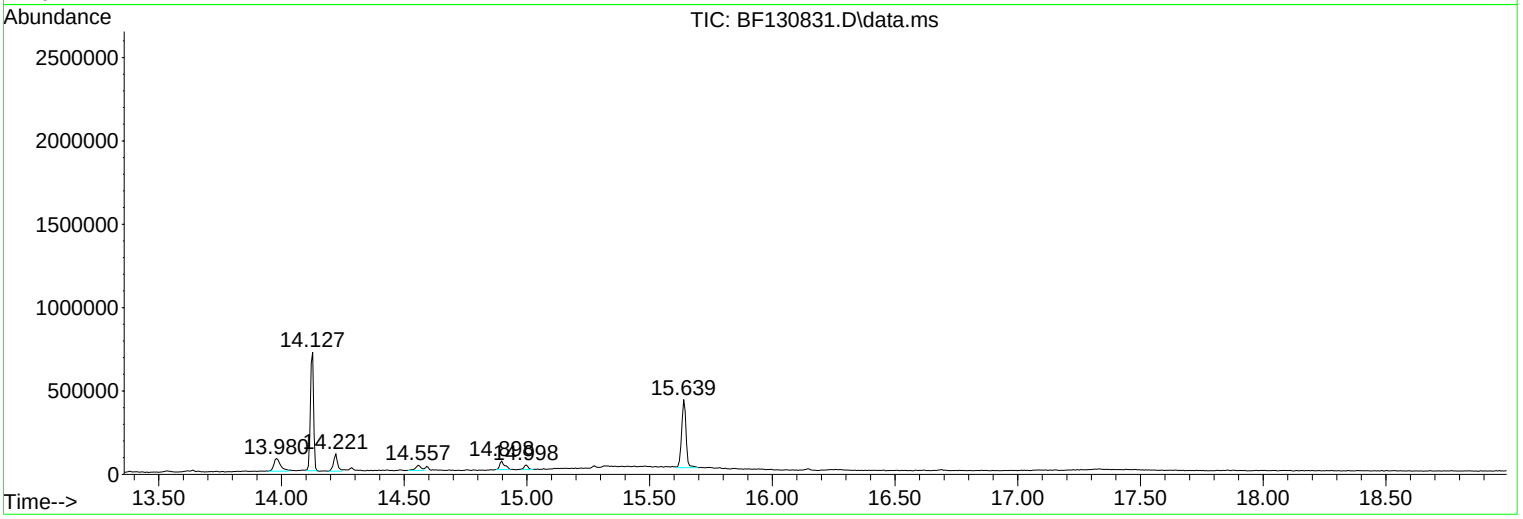
ClientSampleId :
SB-12

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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

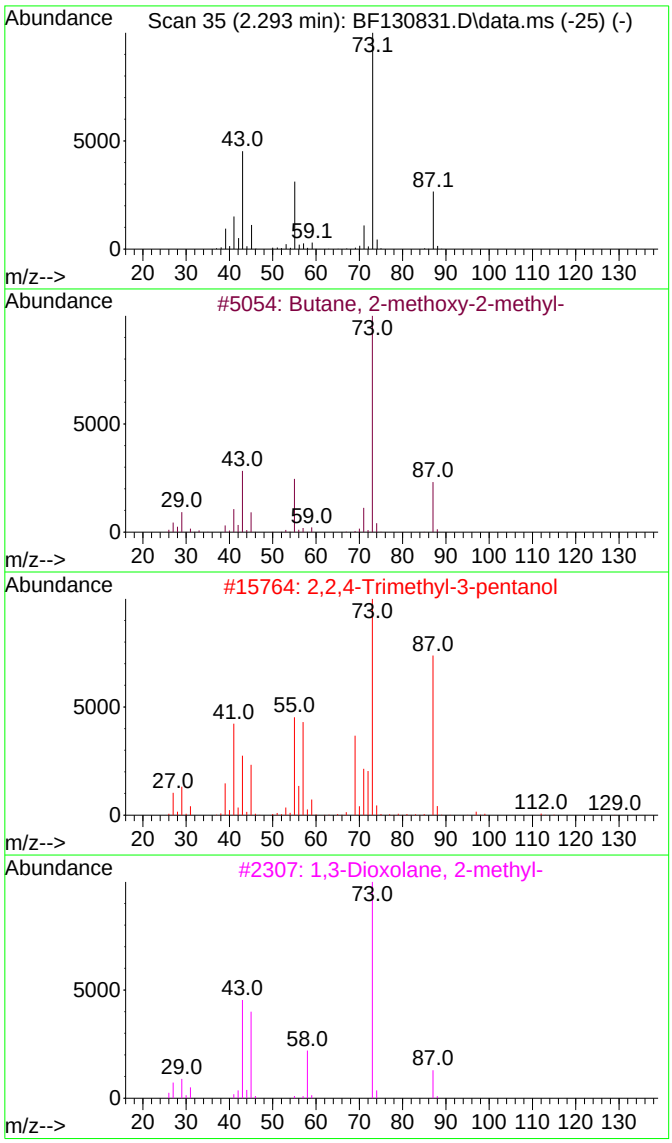
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

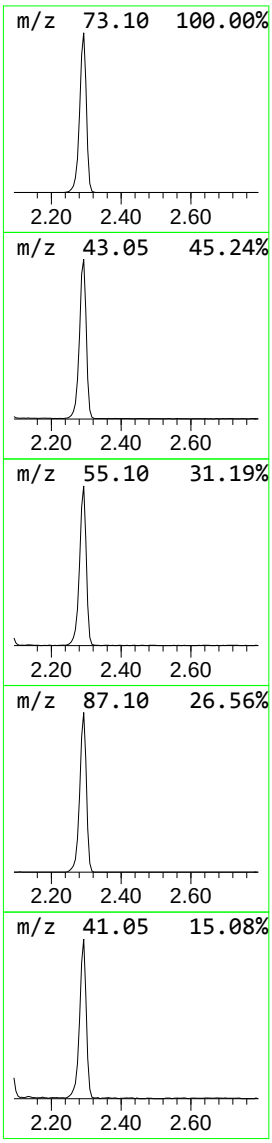
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.293	49.95 ng	1532480	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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9





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Operator : CG\JU
Sample : N5281-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

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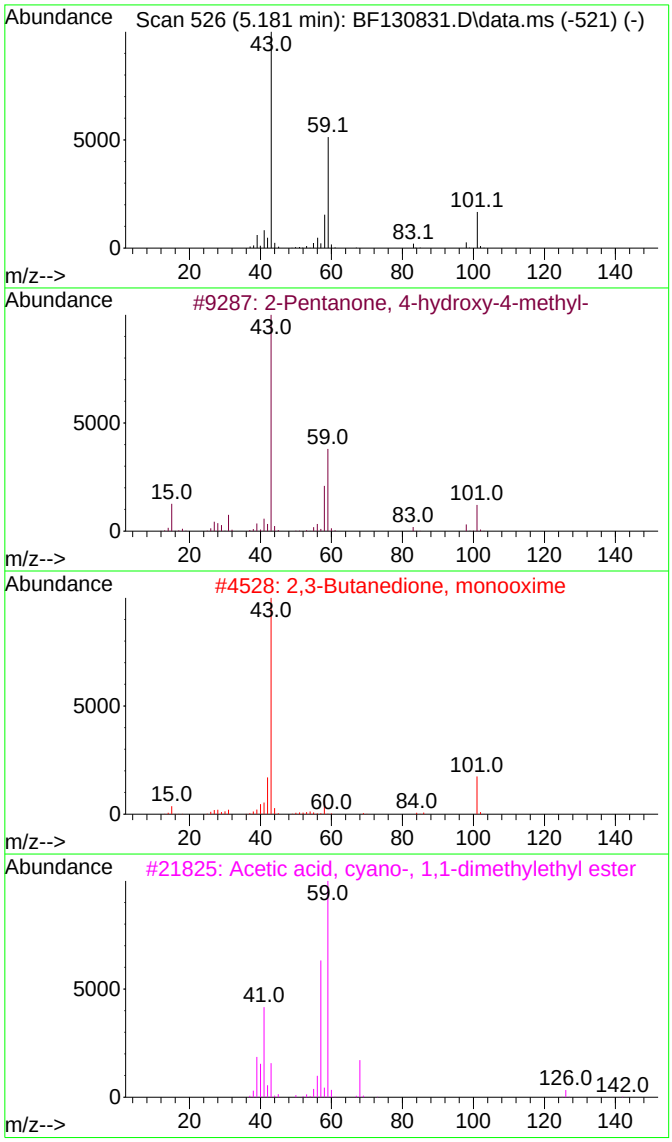
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

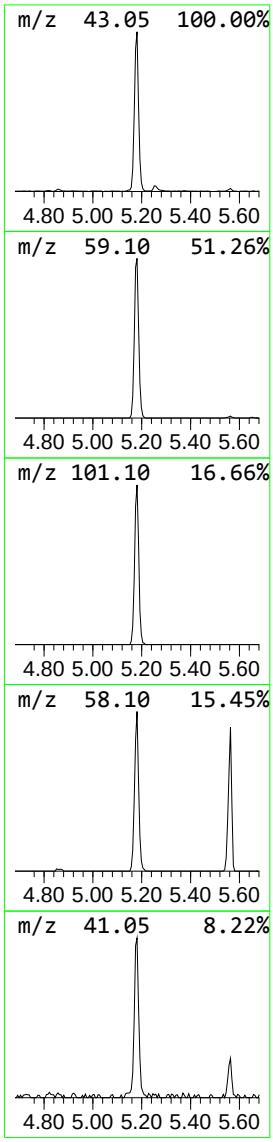
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.181	11.10 ng	340472	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	59
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	Ethanol, pentamethyl-	116	C7H16O	000594-83-2	9





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Operator : CG\JU
Sample : N5281-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

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

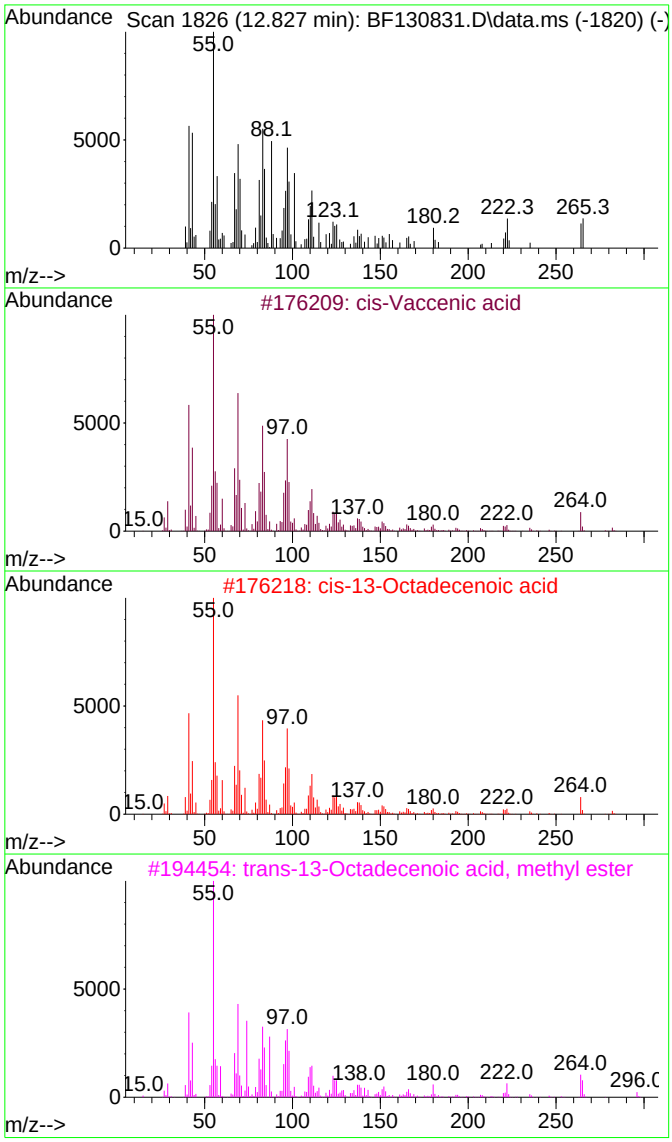
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

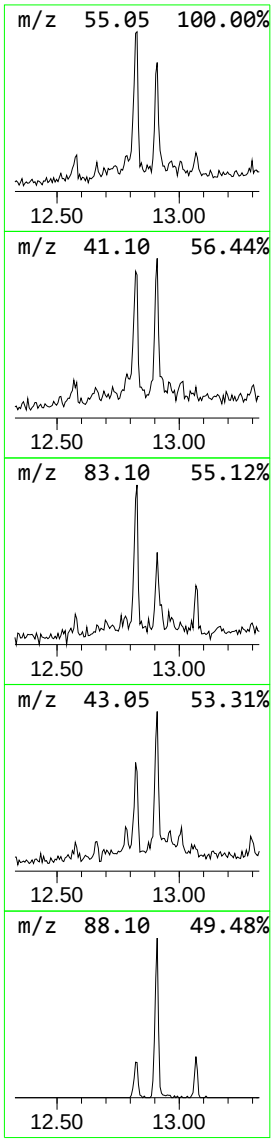
****

Peak Number 3 cis-Vaccenic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.827	3.59 ng	116291	Chrysene-d12	14.127

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-Vaccenic acid	282	C18H34O2	000506-17-2	60
2	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	58
3	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	58
4	trans-9-Octadecenoic acid, penty...	352	C23H44O2	1000405-19-1	58
5	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	53





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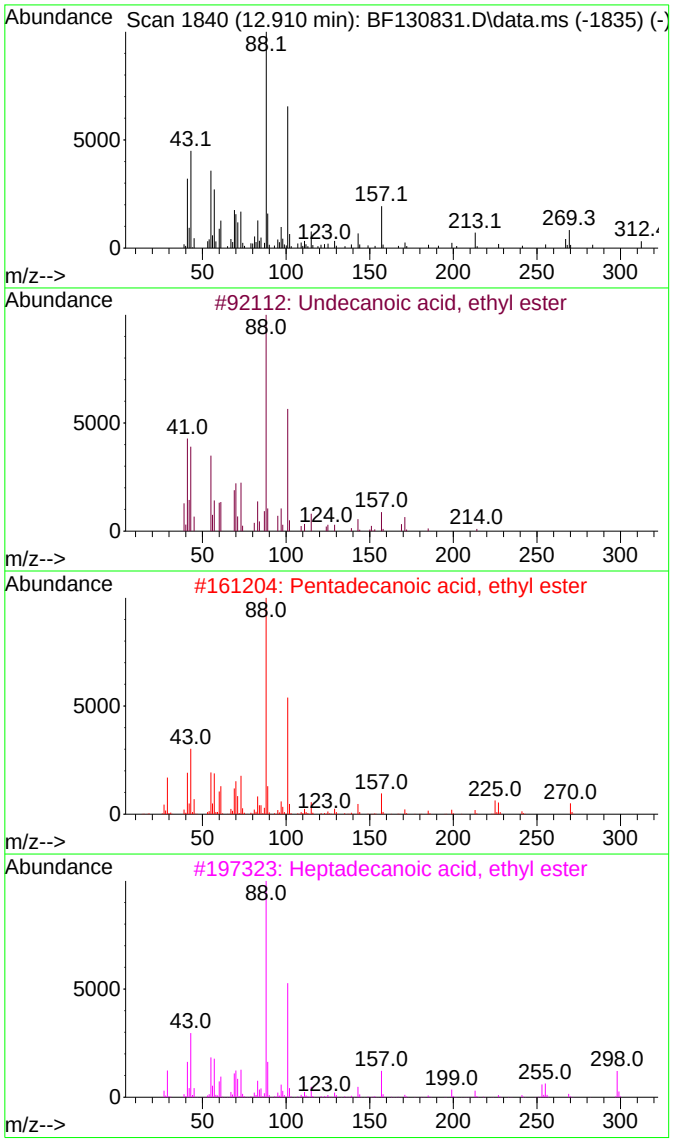
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

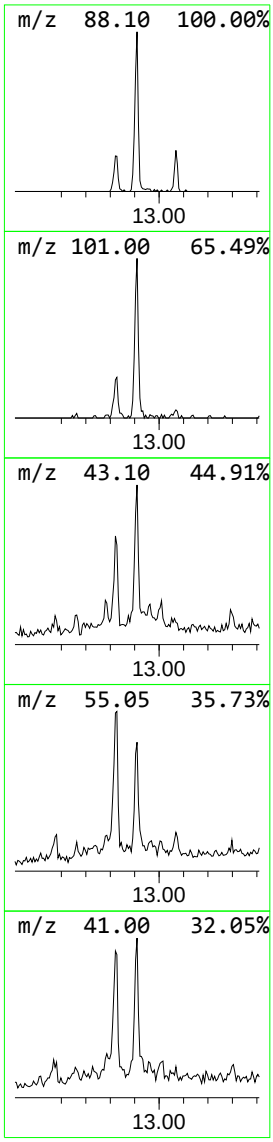
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Undecanoic acid, ethyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.910	3.62 ng	117194	Chrysene-d12	14.127

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid, ethyl ester	214	C13H26O2	000627-90-7	91
2	Pentadecanoic acid, ethyl ester	270	C17H34O2	041114-00-5	91
3	Heptadecanoic acid, ethyl ester	298	C19H38O2	014010-23-2	86
4	Hexadecanoic acid, ethyl ester	284	C18H36O2	000628-97-7	86
5	Eicosanoic acid, ethyl ester	340	C22H44O2	018281-05-5	83





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Sample : N5281-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

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

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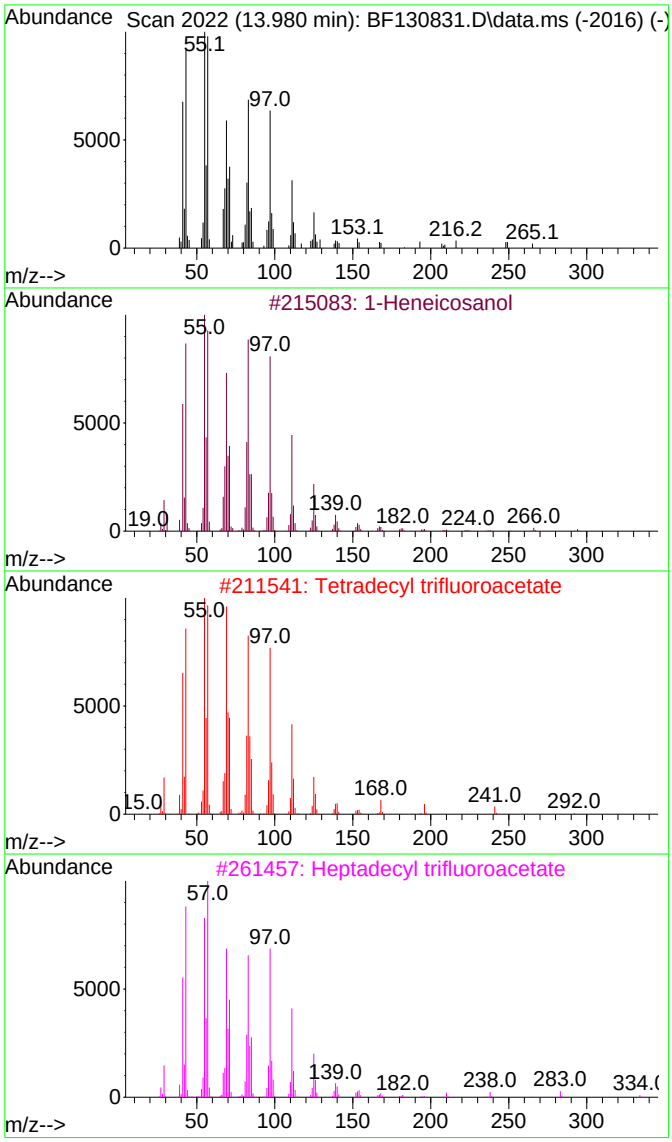
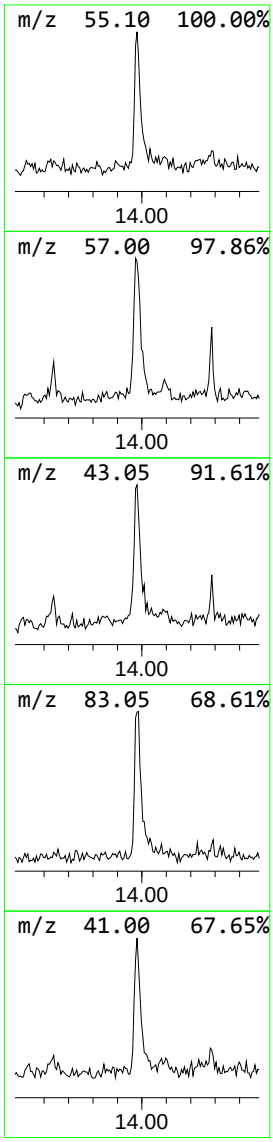
Peak Number 5 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.980	4.58 ng	148432	Chrysene-d12	14.127

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	94
2	Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	91
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91
4	Pentafluoropropionic acid, tride...	346	C16H27F5O2	959261-22-4	91
5	1-Octadecanol	270	C18H38O	000112-92-5	91





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Sample : N5281-13
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

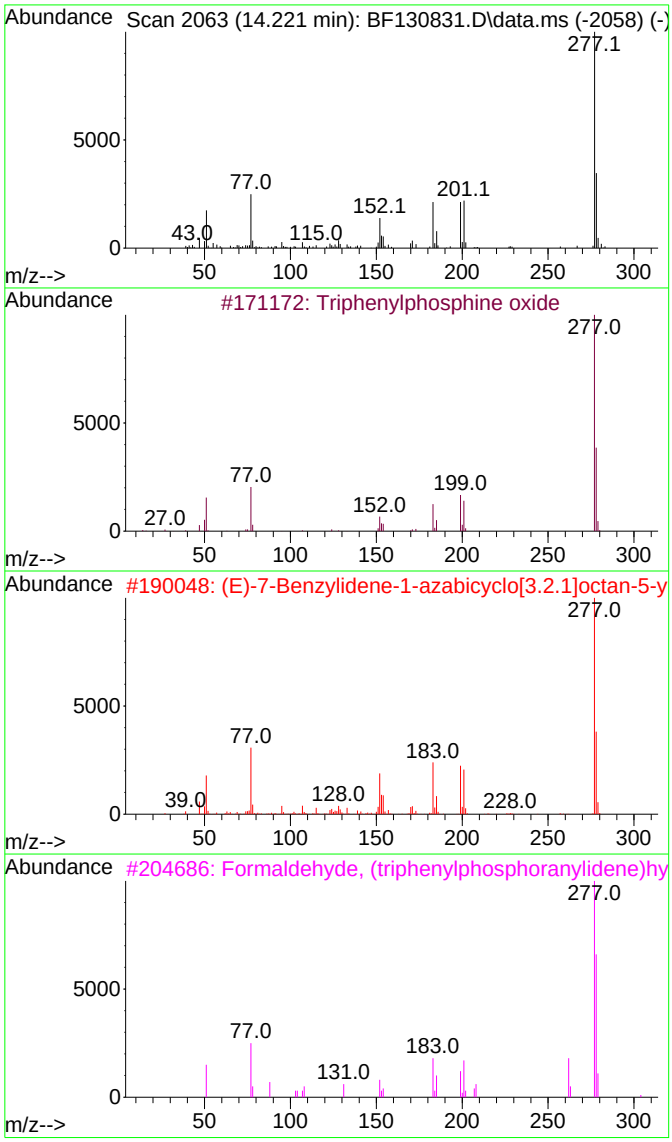
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

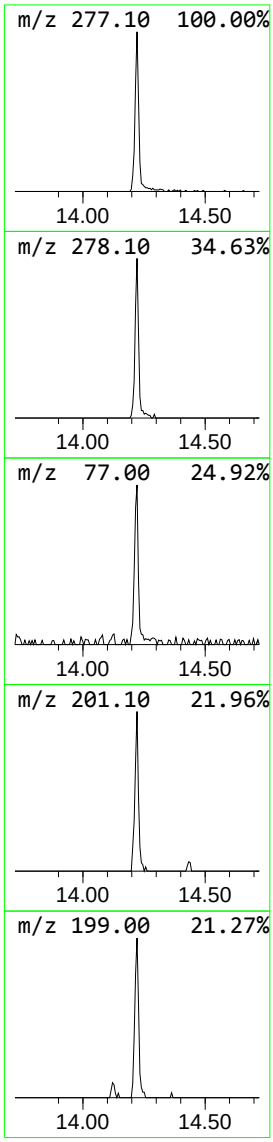
****

Peak Number 6 Triphenylphosphine oxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.221	3.58 ng	116210	Chrysene-d12	14.127

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	95
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	90
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	38
4	1H-Indole-3-acetic acid, 5-[(tri...	277	C14H19NO3Si	072101-35-0	17
5	[1,2,4]Triazolo[1,5-a]pyrimidine...	278	C15H14N6	1000350-69-0	9





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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

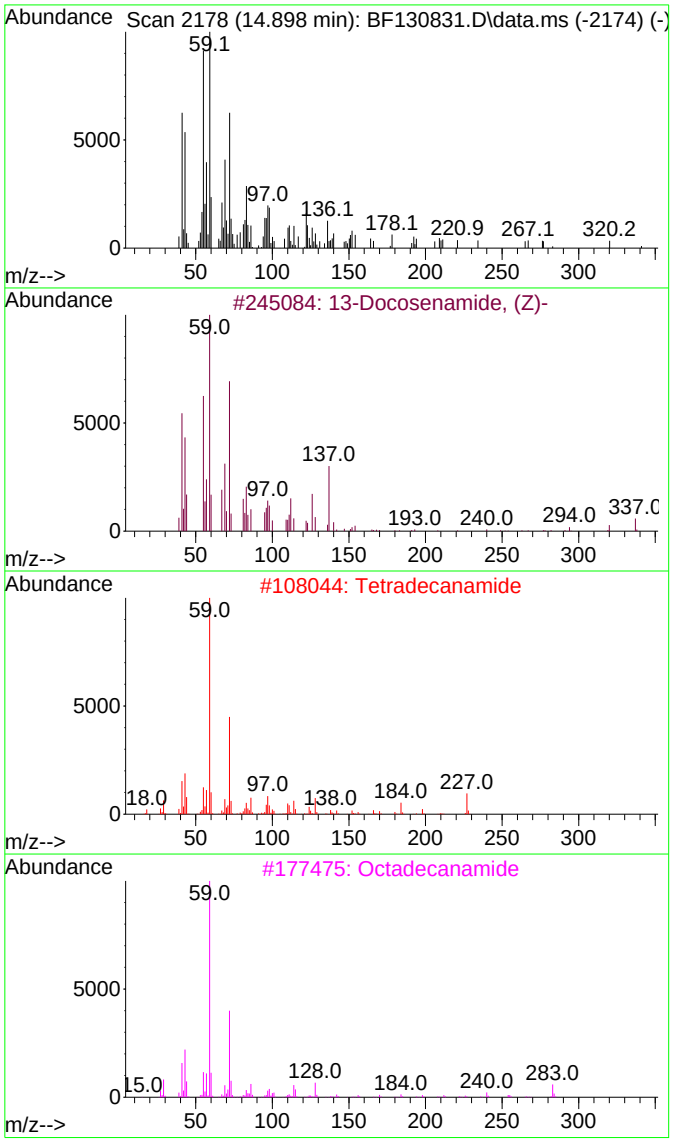
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

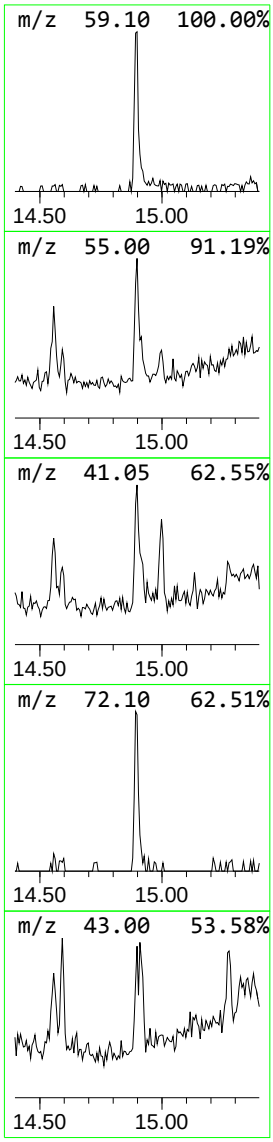
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.898	2.89 ng	73479	Perylene-d12	15.639

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	59
2	Tetradecanamide	227	C14H29NO	000638-58-4	59
3	Octadecanamide	283	C18H37NO	000124-26-5	53
4	Hexadecanamide	255	C16H33NO	000629-54-9	50
5	1-Cyclohexyl-2-methyl-2-propanol	156	C10H20O	005531-30-6	27





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.293	50.0	ng	1532480	1	6.945	613579	20.0
2-Pentanone, 4-...	5.181	11.1	ng	340472	1	6.945	613579	20.0
cis-Vaccenic acid	12.827	3.6	ng	116291	5	14.127	648319	20.0
Undecanoic acid...	12.910	3.6	ng	117194	5	14.127	648319	20.0
1-Heneicosanol	13.980	4.6	ng	148432	5	14.127	648319	20.0
Triphenylphosph...	14.221	3.6	ng	116210	5	14.127	648319	20.0
13-Docosenamide...	14.898	2.9	ng	73479	6	15.639	508761	20.0