LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110122\
Data File : BF130907.D
Acq On : 01 Nov 2022 18:53
Operator : CG\JU
Sample : N5380-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-D

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: BF130907.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.252	21	28	33	rVB	510538	655525	31.13%	4.495%
2	2.363	41	47	56	rVB	40024	58768	2.79%	0.403%
3	5.163	518	523	532	rVB	286787	328895	15.62%	2.255%
4	5.551	584	589	592	rBV	1976170	1877084	89.13%	12.871%
5	6.551	754	759	762	rBV	1776678	1916586	91.00%	13.142%
6	6.934	820	824	827	rBV	759957	581123	27.59%	3.985%
7	7.498	914	920	923	rBV	1353634	1241409	58.94%	8.512%
8	8.116	1021	1025	1038	rBV	189646	293623	13.94%	2.013%
9	8.216	1038	1042	1046	rVB	819949	733305	34.82%	5.028%
10	9.298	1220	1226	1229	rBV	2598563	2106102	100.00%	14.441%
11	9.981	1338	1342	1345	rBV	937023	718463	34.11%	4.926%
12	10.769	1472	1476	1479	rBV	1174525	942874	44.77%	6.465%
13	11.475	1592	1596	1599	rBV	652490	568368	26.99%	3.897%
14	11.857	1658	1661	1664	rBV2	33247	29449	1.40%	0.202%
15	11.986	1680	1683	1690	rBV	69272	77550	3.68%	0.532%
16	13.063	1862	1866	1869	rBV	1625126	1310462	62.22%	8.986%
17	14.121	2042	2046	2051	rVB	557111	475127	22.56%	3.258%
18	14.216	2059	2062	2067	rVB	47876	47429	2.25%	0.325%
19	14.886	2173	2176	2182	rBV2	144901	173784	8.25%	1.192%
20	14.986	2191	2193	2196	rVB	52149	44698	2.12%	0.306%
21	15.639	2299	2304	2312	rVB	289615	403244	19.15%	2.765%

Sum of corrected areas: 14583868

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110122\
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Misc :
ALS Vial : 7 Sample Multiplier: 1

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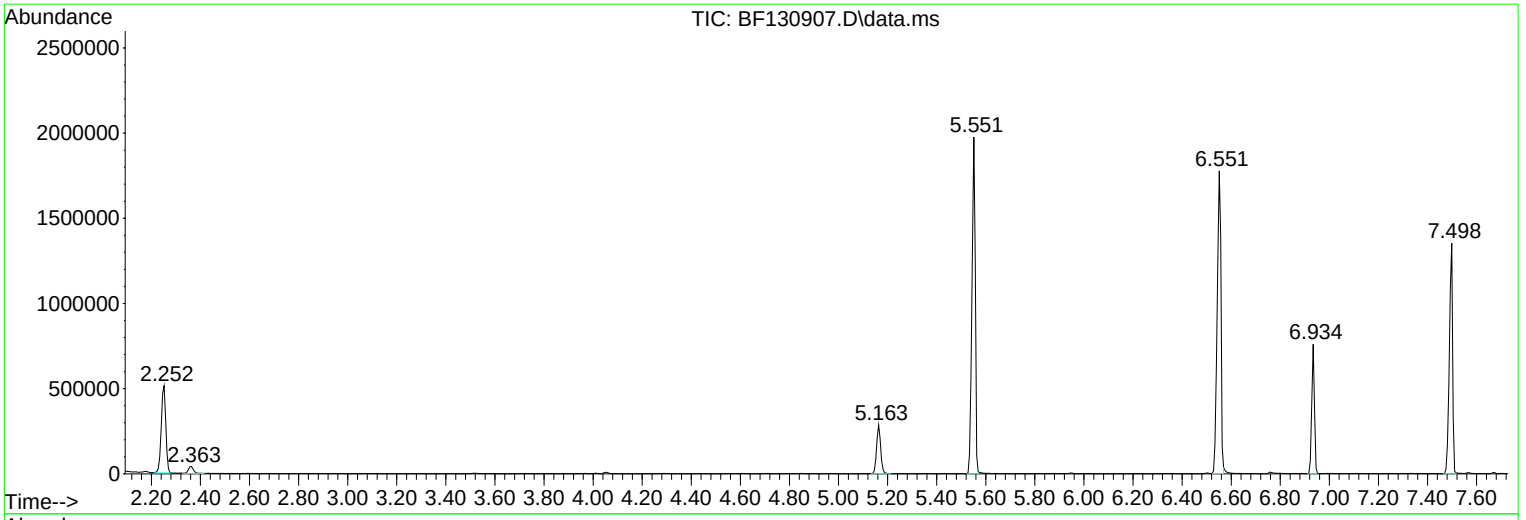
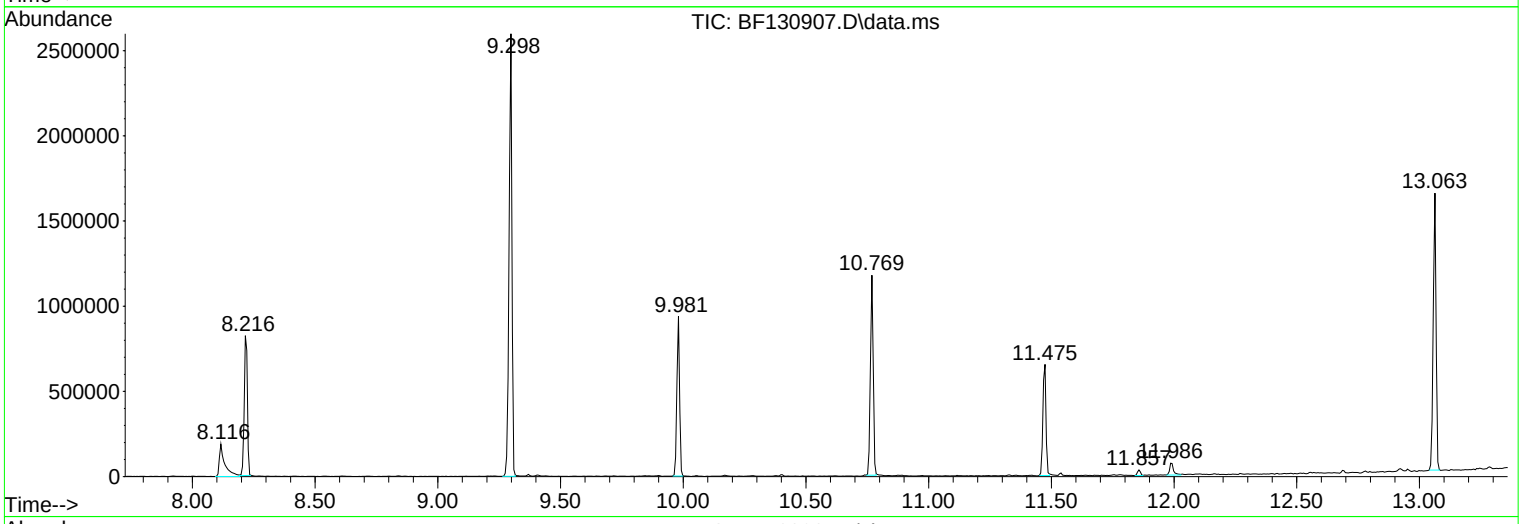
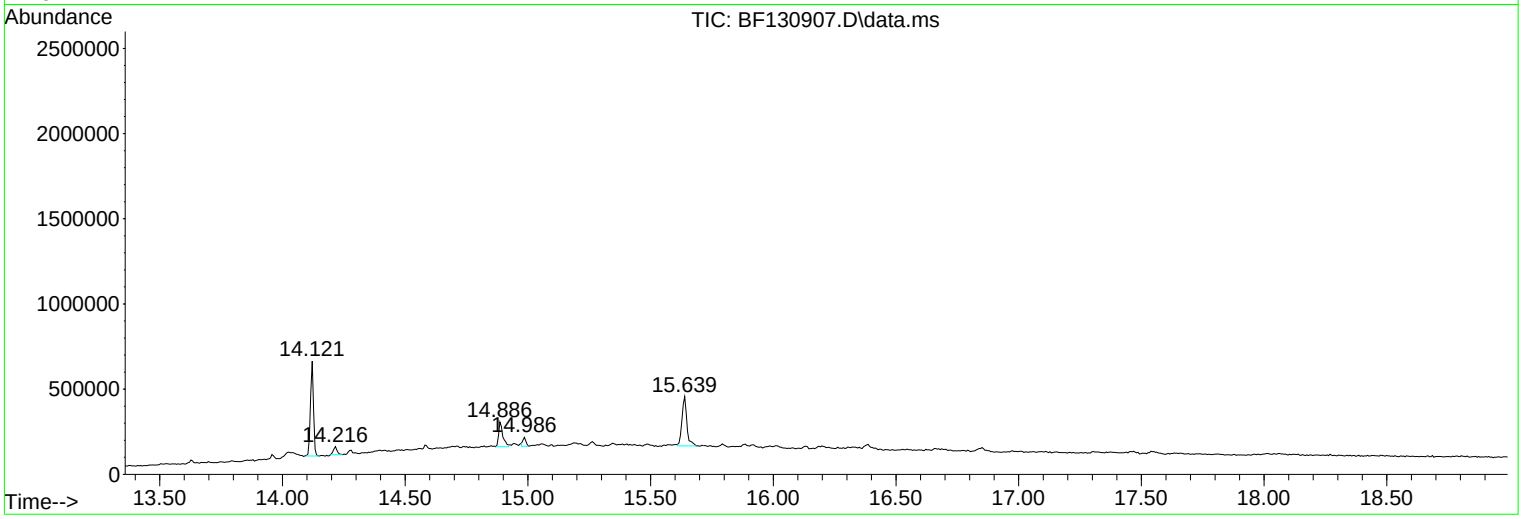
BNA_F
ClientSampleId :
TP-D

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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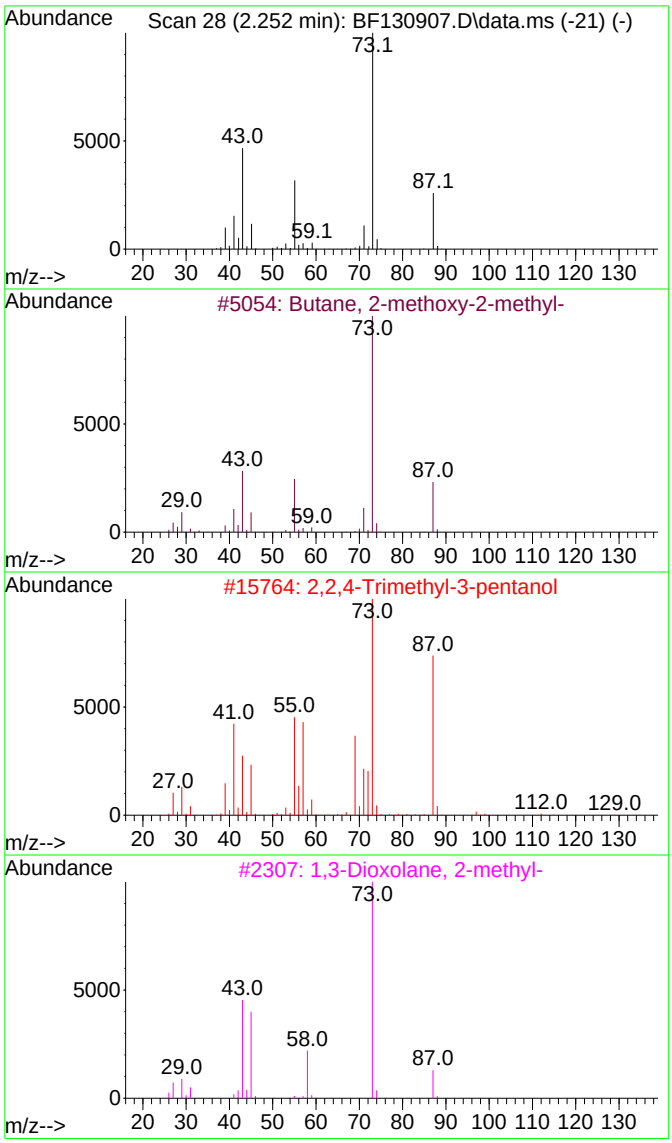
TIC Integration Parameters: LSCINT.P

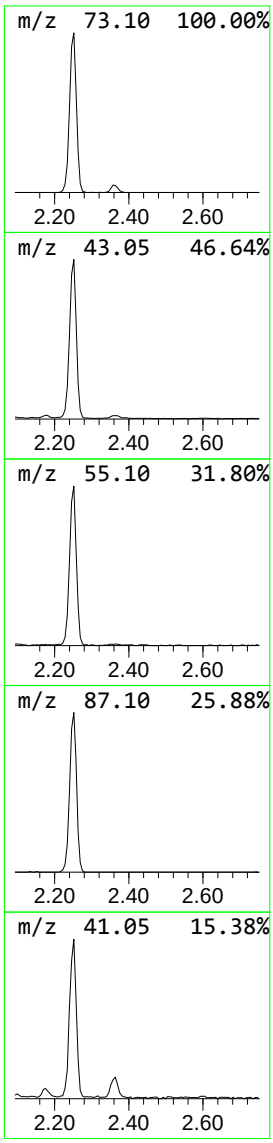
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.252	22.56 ng	655525	1,4-Dichlorobenzene-d4	6.934

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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





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TP-D

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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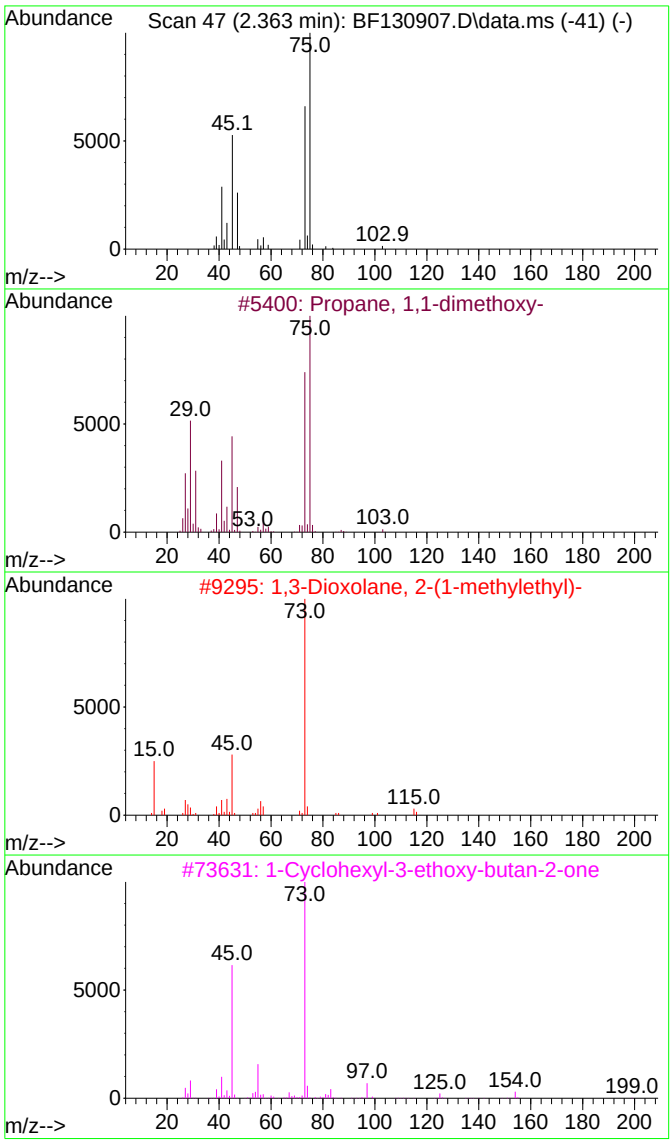
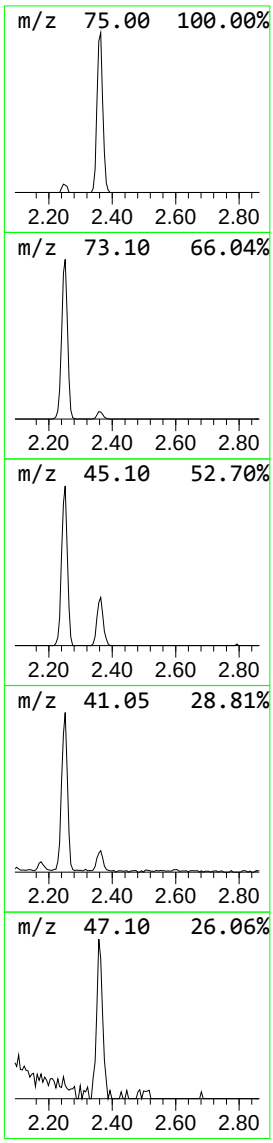
Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.363	2.02 ng	58768	1,4-Dichlorobenzene-d4	6.934

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	9
3	1-Cyclohexyl-3-ethoxy-butan-2-one	198	C12H22O2	074897-69-1	9
4	5-Hexen-2-ol	100	C6H12O	000626-94-8	9
5	Silanol, trimethyl-	90	C3H10OSi	001066-40-6	9





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Sample : N5380-04
Misc :
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Instrument :
BNA_F
ClientSampleId :
TP-D

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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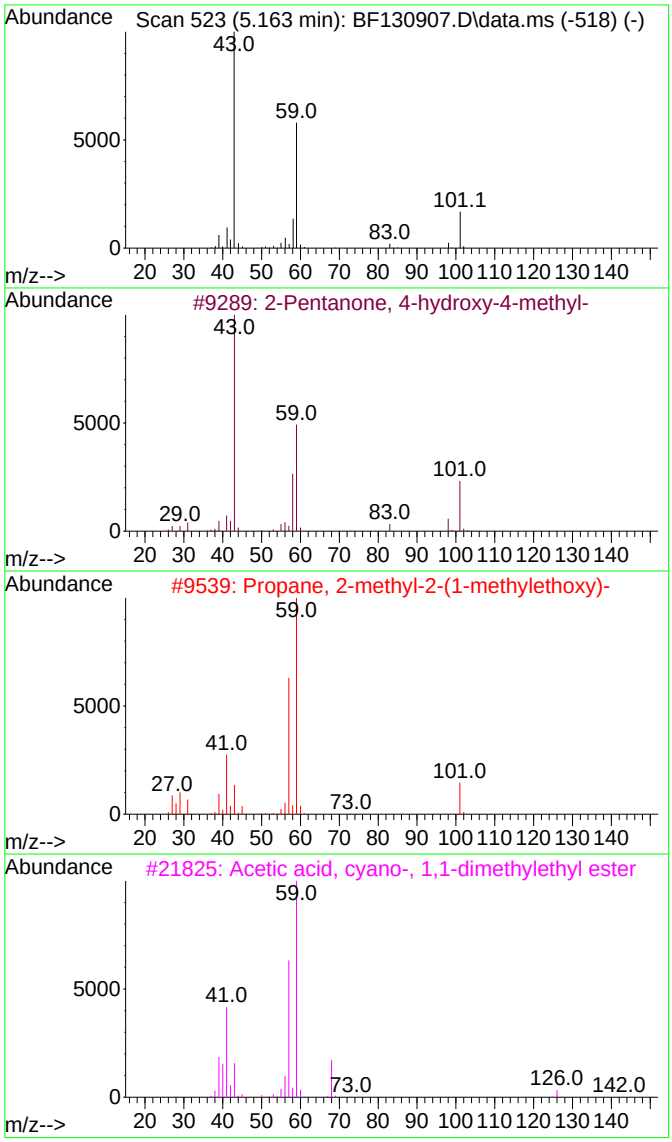
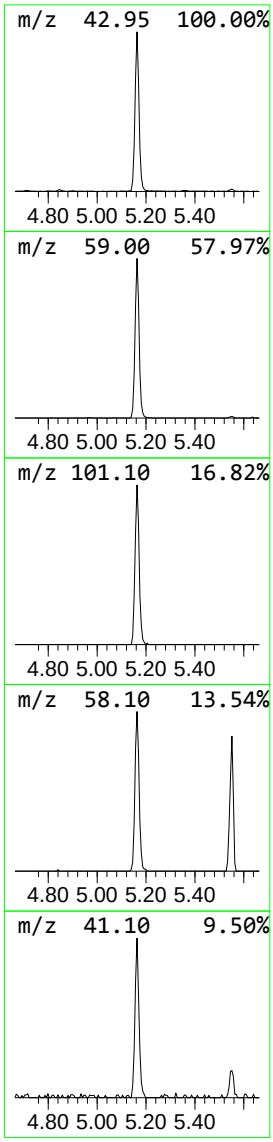
Peak Number 3 unknown5.163 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.163	11.32 ng	328895	1,4-Dichlorobenzene-d4	6.934

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	47
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
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	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Sample : N5380-04
Misc :
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Instrument :
BNA_F
ClientSampleId :
TP-D

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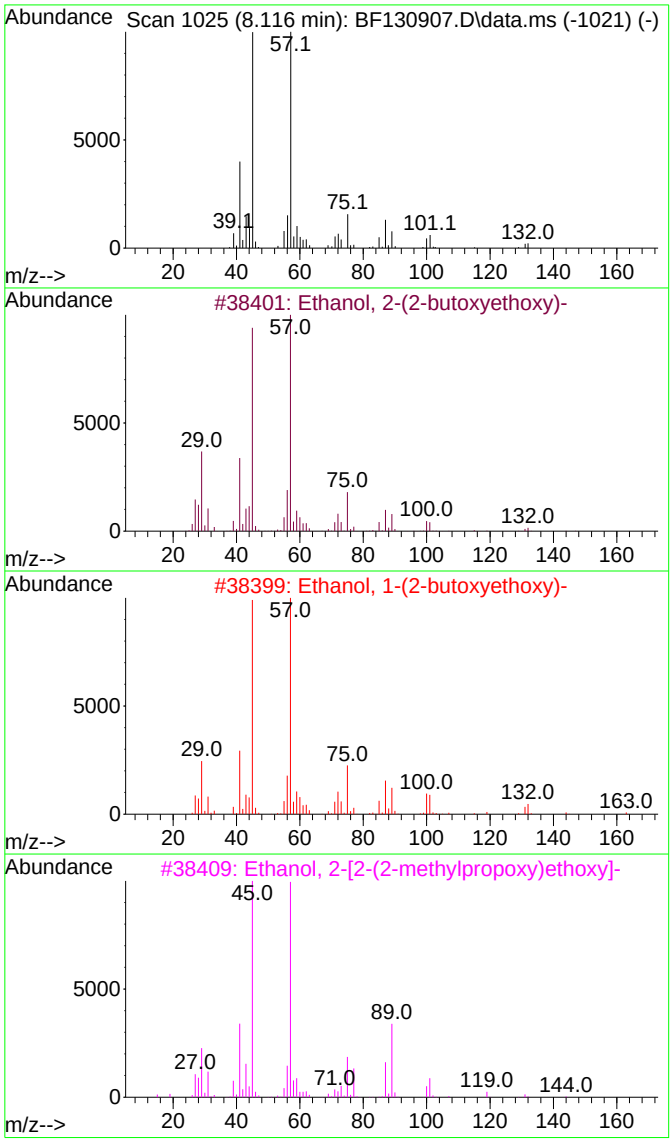
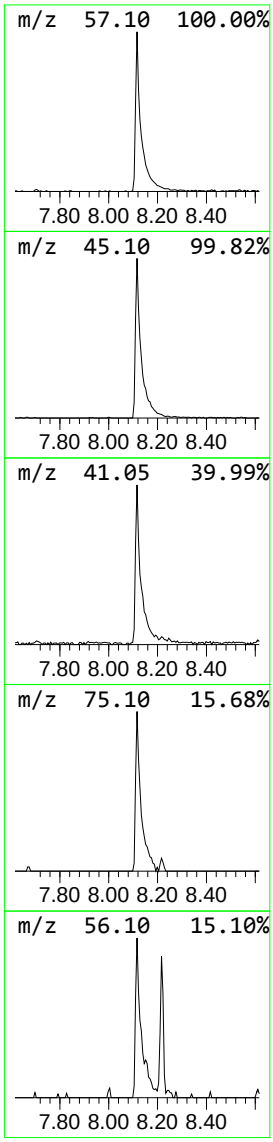
Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.116	8.01 ng	293623	Naphthalene-d8	8.216

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	90
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	78
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
5	Tetraethylene glycol	194	C8H18O5	000112-60-7	50





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BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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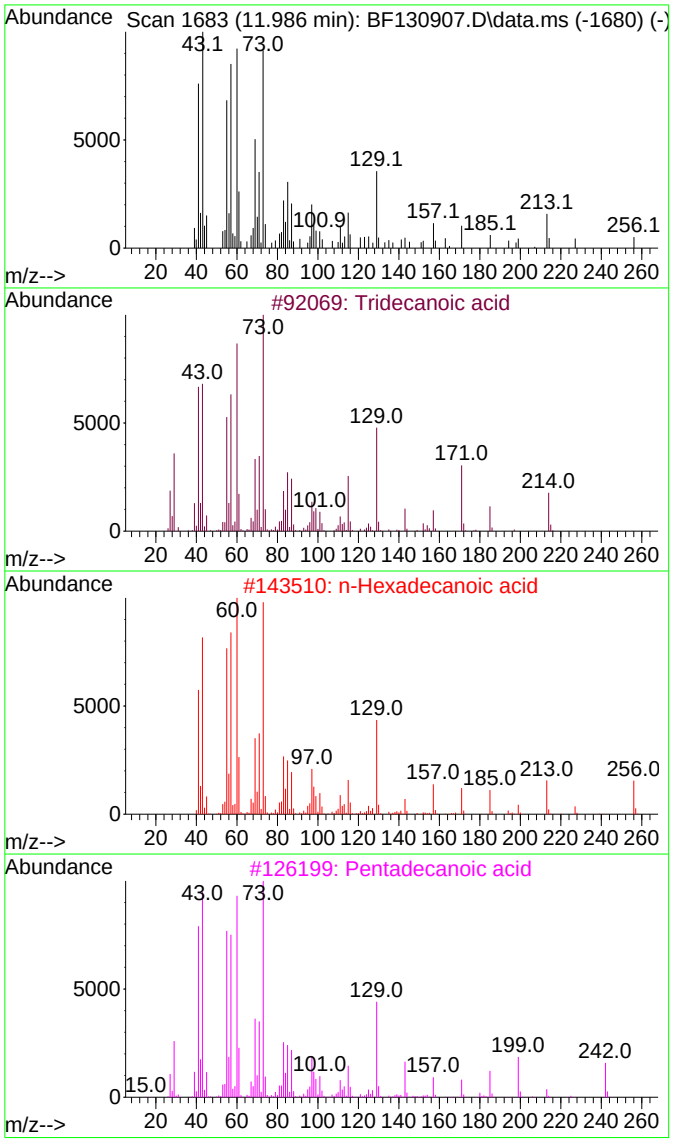
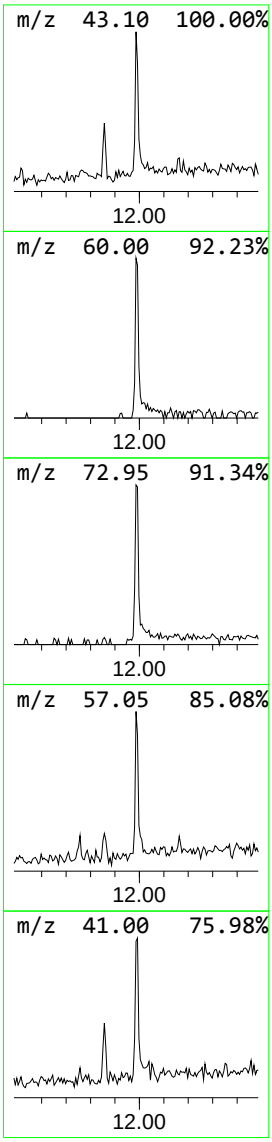
Peak Number 5 Tridecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.986	2.73 ng	77550	Phenanthrene-d10	11.475

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	95
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5	Nonanoic acid	158	C9H18O2	000112-05-0	49





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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
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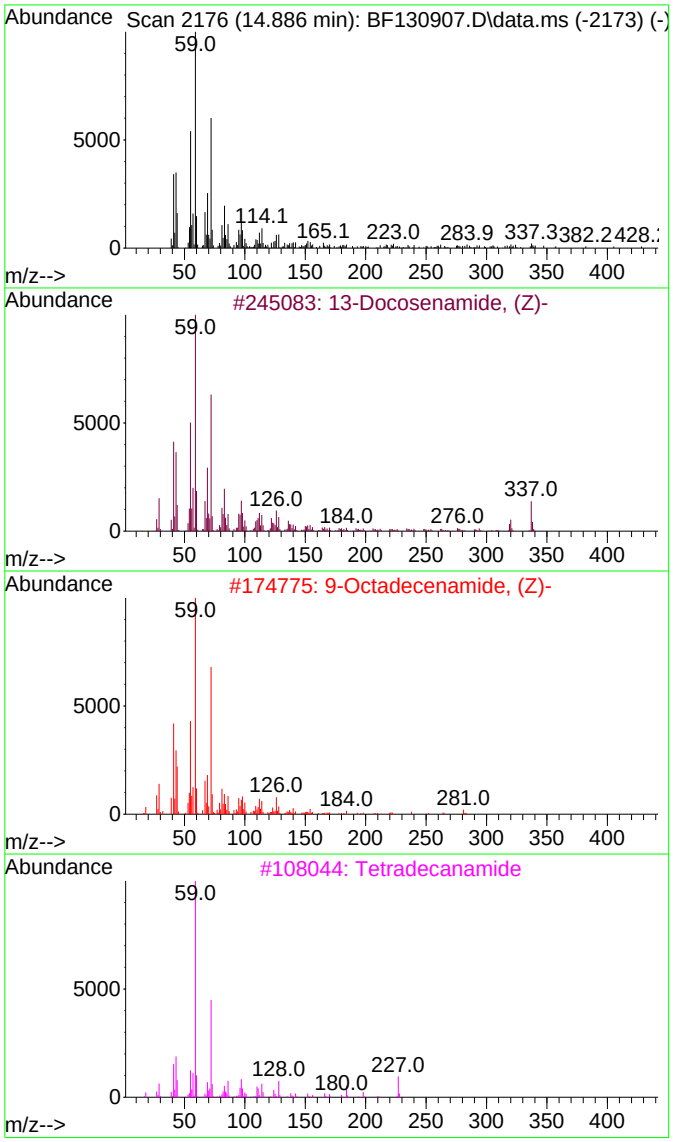
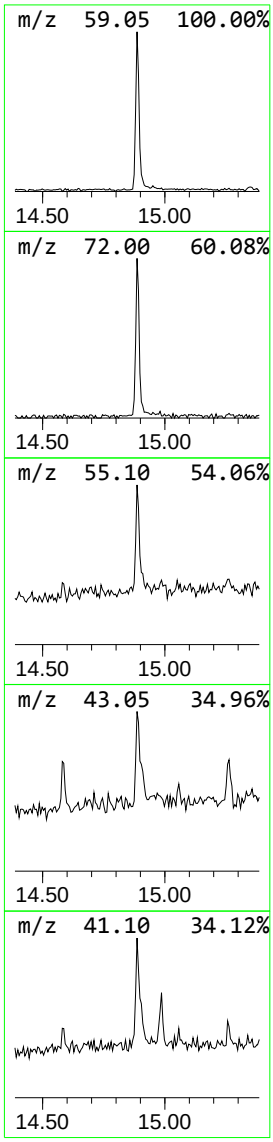
Peak Number 6 13-Docosenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.886	8.62 ng	173784	Perylene-d12	15.639

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	74
3	Tetradecanamide	227	C14H29NO	000638-58-4	72
4	Dodecanamide	199	C12H25NO	001120-16-7	58
5	7-Nonenamide	155	C9H17NO	090949-53-4	53





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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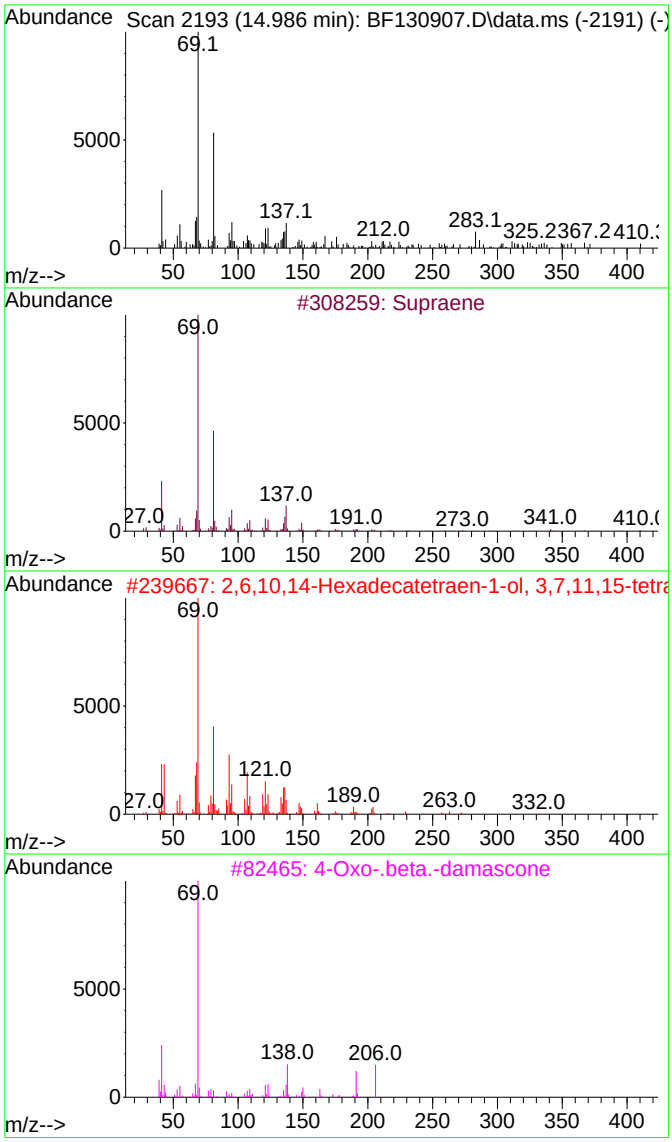
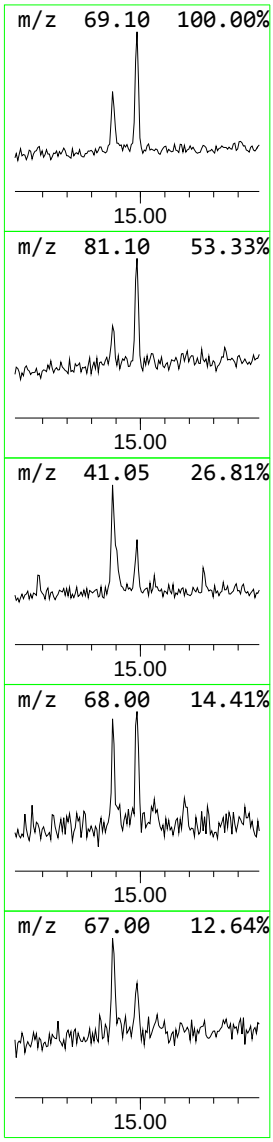
Peak Number 7 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.986	2.22 ng	44698	Perylene-d12	15.639

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	80
2	2,6,10,14-Hexadecatetraen-1-ol, ...	332	C22H36O2	061691-98-3	64
3	4-Oxo-.beta.-damascone	206	C13H18O2	053398-08-6	64
4	4,8,12-Tetradecatrienenitrile, 5...	245	C17H27N	005981-31-7	64
5	3,7-Dimethyl-1-phenylsulfonyl-2,...	278	C16H22O2S	1000432-27-5	59





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...	2.252	22.6	ng	655525	1	6.934	581123	20.0
Propane, 1,1-di...	2.363	2.0	ng	58768	1	6.934	581123	20.0
unknown5.163	5.163	11.3	ng	328895	1	6.934	581123	20.0
Ethanol, 2-(2-b...	8.116	8.0	ng	293623	2	8.216	733305	20.0
Tridecanoic acid	11.986	2.7	ng	77550	4	11.475	568368	20.0
13-Docosenamide...	14.886	8.6	ng	173784	6	15.639	403244	20.0
Supraene	14.986	2.2	ng	44698	6	15.639	403244	20.0