LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
Data File : BF126937.D
Acq On : 17 Feb 2022 20:14
Operator : CG\JU
Sample : N1573-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-20R

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-BF021622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126937.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.457	365	369	379	rVB	352159	412432	8.14%	1.547%
2	5.157	484	488	495	rBV	130137	154679	3.05%	0.580%
3	5.545	549	554	557	rBV	2116196	1900896	37.53%	7.131%
4	6.539	719	723	727	rBV	1293556	1229550	24.27%	4.613%
5	6.722	751	754	756	rBV	242342	176812	3.49%	0.663%
6	6.751	756	759	762	rVB	244430	189829	3.75%	0.712%
7	6.839	771	774	785	rBV	318482	304049	6.00%	1.141%
8	6.928	785	789	792	rBV	862848	657163	12.97%	2.465%
9	6.981	795	798	808	rVB	148148	129648	2.56%	0.486%
10	7.498	877	886	888	rBV	2445344	2752385	54.34%	10.326%
11	7.563	893	897	901	rBV	59613	70309	1.39%	0.264%
12	8.110	986	990	997	rBV2	81884	110292	2.18%	0.414%
13	8.210	1003	1007	1010	rBV	1149004	916274	18.09%	3.437%
14	8.357	1029	1032	1040	rBV	74724	77021	1.52%	0.289%
15	8.610	1072	1075	1082	rVB2	42013	51545	1.02%	0.193%
16	9.157	1164	1168	1173	rBV	261346	267860	5.29%	1.005%
17	9.286	1184	1190	1193	rBV	4741370	5065517	100.00%	19.004%
18	9.380	1202	1206	1209	rBV	1086798	830171	16.39%	3.114%
19	9.710	1258	1262	1267	rVB4	37449	50951	1.01%	0.191%
20	9.969	1303	1306	1309	rVB	1262531	971421	19.18%	3.644%
21	10.274	1354	1358	1361	rBV2	68875	57812	1.14%	0.217%
22	10.380	1372	1376	1379	rVB	212984	174974	3.45%	0.656%
23	10.669	1422	1425	1427	rBV	222434	169265	3.34%	0.635%
24	10.763	1436	1441	1444	rBV	3399720	3172490	62.63%	11.902%
25	11.457	1555	1559	1562	rBV	1255207	1026993	20.27%	3.853%
26	11.833	1620	1623	1627	rBV	195355	151337	2.99%	0.568%
27	13.051	1824	1830	1833	rBV	4591064	4508778	89.01%	16.915%
28	14.098	2004	2008	2012	rBV	643940	537948	10.62%	2.018%
29	15.604	2258	2264	2272	rBV	423777	537158	10.60%	2.015%

Sum of corrected areas: 26655559

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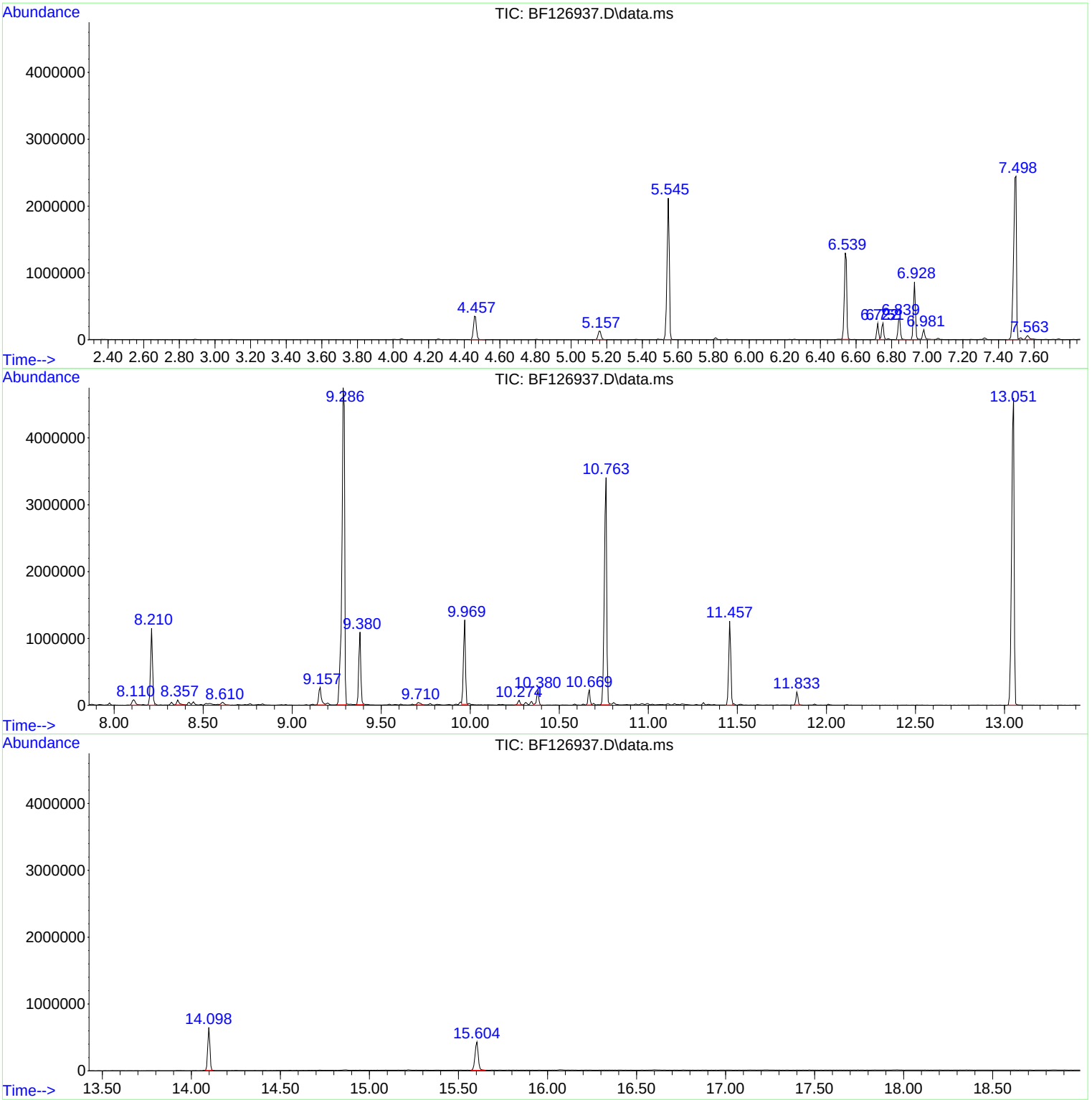
Instrument :
BNA_F
ClientSampleId :
MW-20R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.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 : BF126937.D
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TIC Library : C:\Database\NIST20.L
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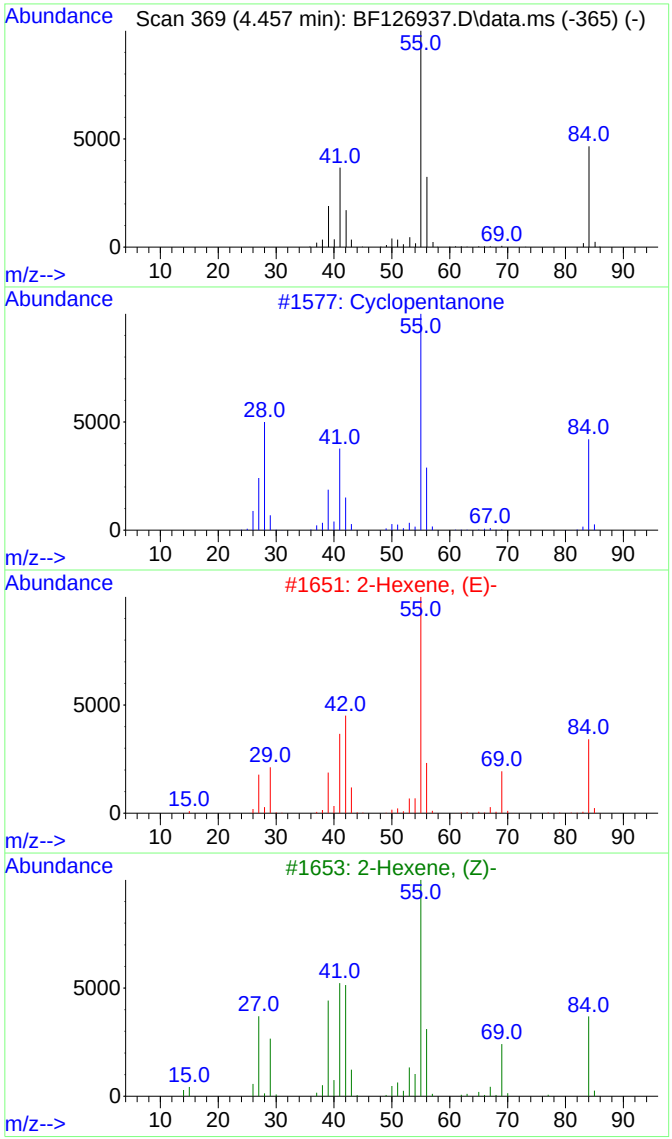
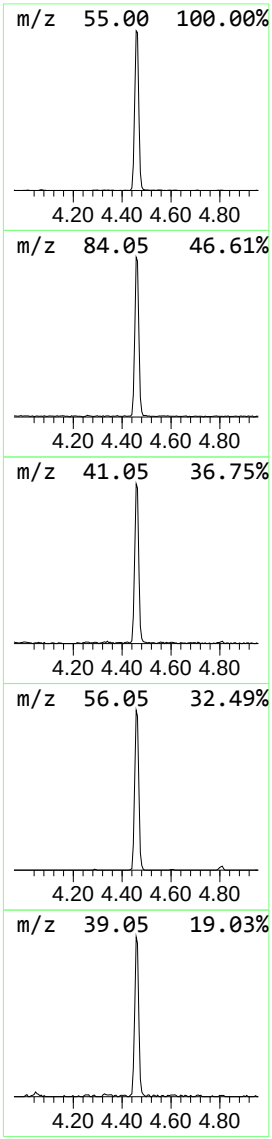
****

Peak Number 1 Cyclopentanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.457	12.55 ng	412432	1,4-Dichlorobenzene-d4	6.928

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanone	84	C5H8O	000120-92-3	91
2	2-Hexene, (E)-	84	C6H12	004050-45-7	59
3	2-Hexene, (Z)-	84	C6H12	007688-21-3	59
4	2-Hexene	84	C6H12	000592-43-8	59
5	3-Hexene, (Z)-	84	C6H12	007642-09-3	53





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Data File : BF126937.D
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Operator : CG\JU
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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-20R

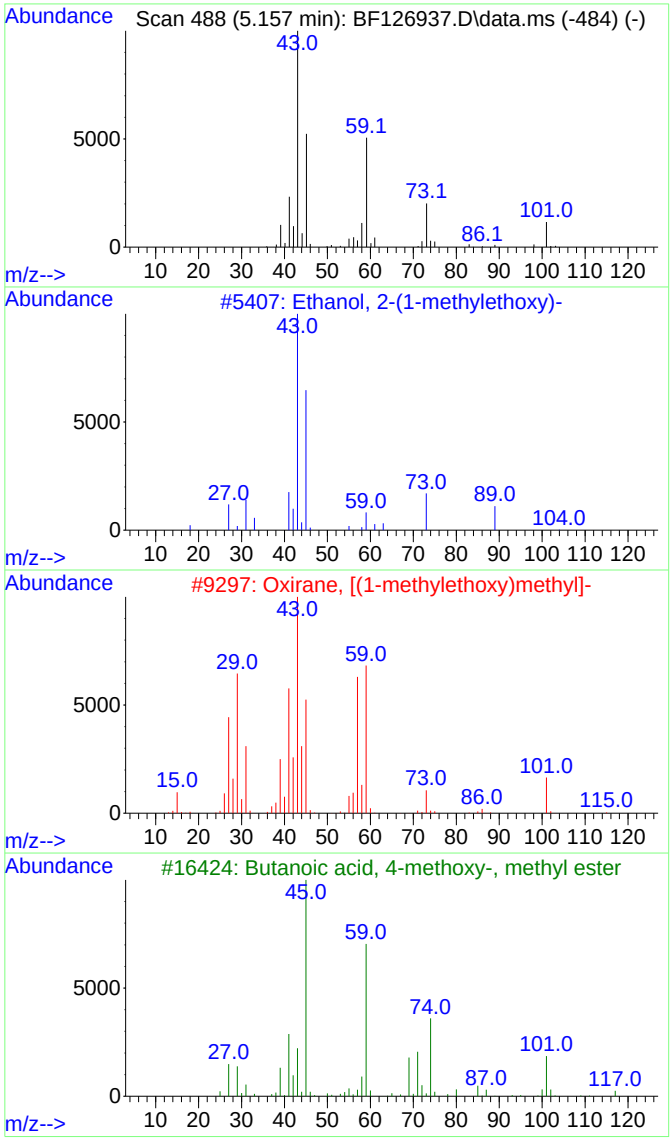
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

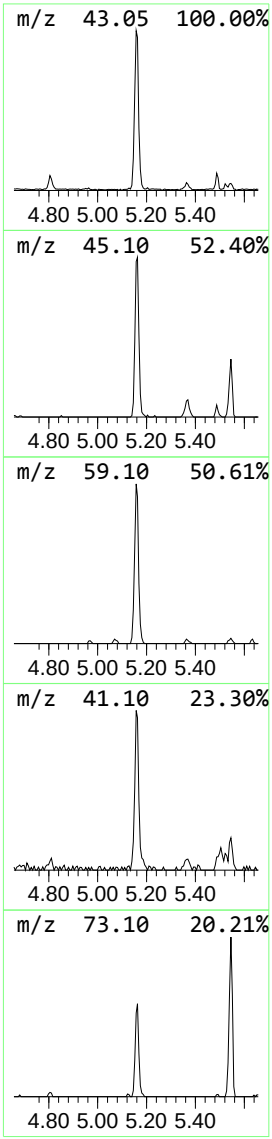
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol, 2-(1-methylethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.157	4.71 ng	154679	1,4-Dichlorobenzene-d4	6.928

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(1-methylethoxy)-	104	C5H12O2	000109-59-1	50
2	Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	50
3	Butanoic acid, 4-methoxy-, methy...	132	C6H12O3	029006-01-7	50
4	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	40
5	Ethanol, 2-propoxy-	104	C5H12O2	002807-30-9	37





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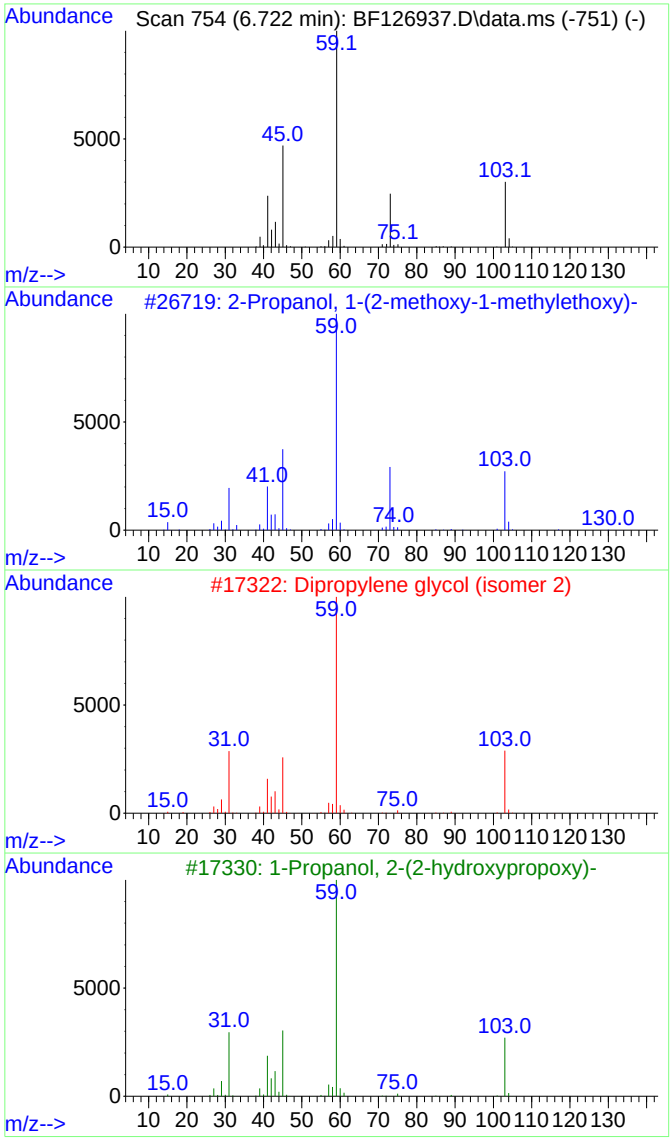
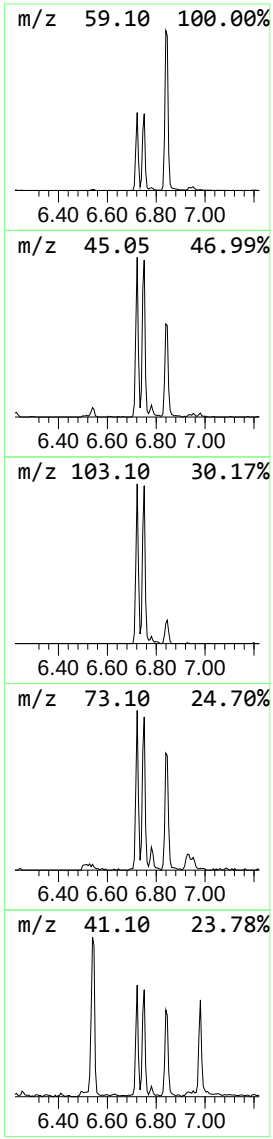
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.722	5.38 ng	176812	1,4-Dichlorobenzene-d4	6.928

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	83
2	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	53
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	53
4	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	53
5	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	40





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ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-20R

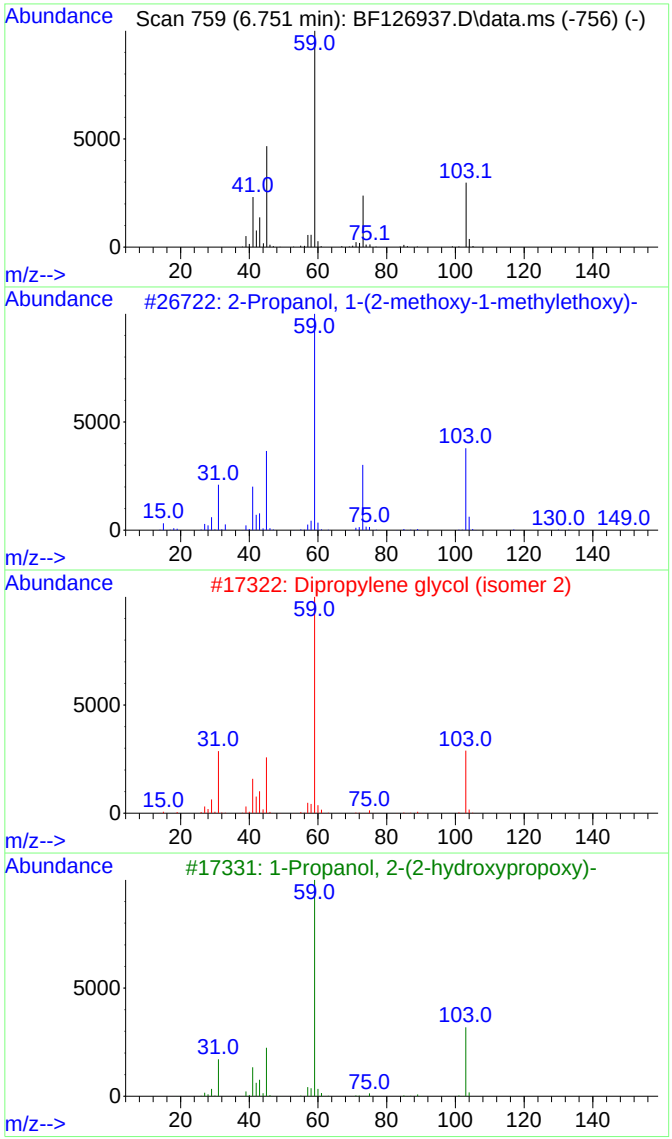
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

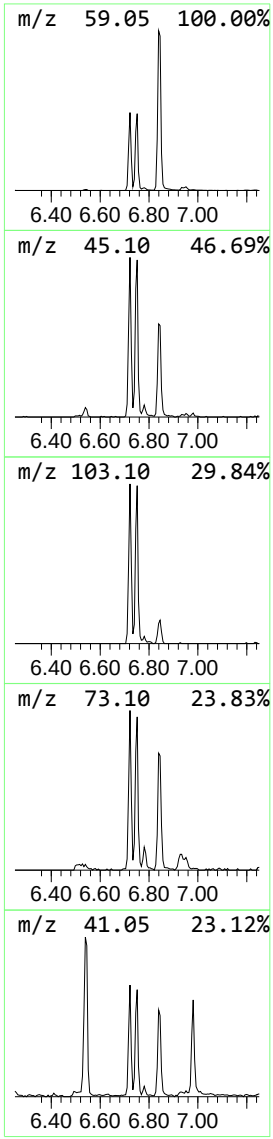
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Dipropylene glycol (isomer 2) Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.751	5.78 ng	189829	1,4-Dichlorobenzene-d4	6.928

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	72
2	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	53
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	50
4	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	50
5	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	50





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Operator : CG\JU
Sample : N1573-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-20R

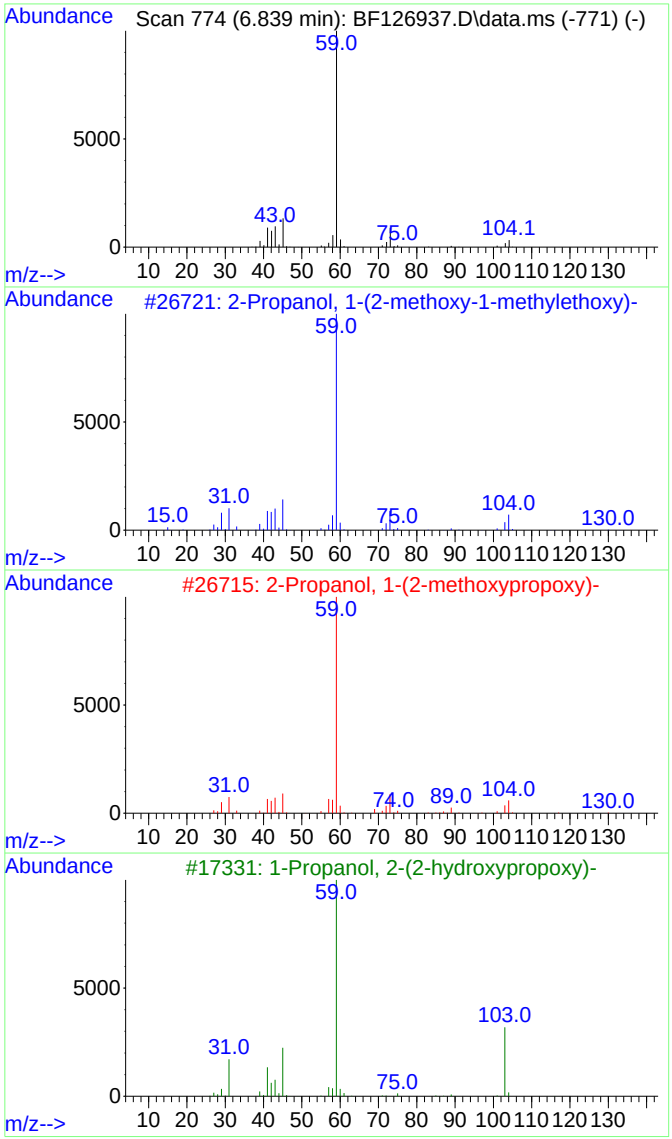
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

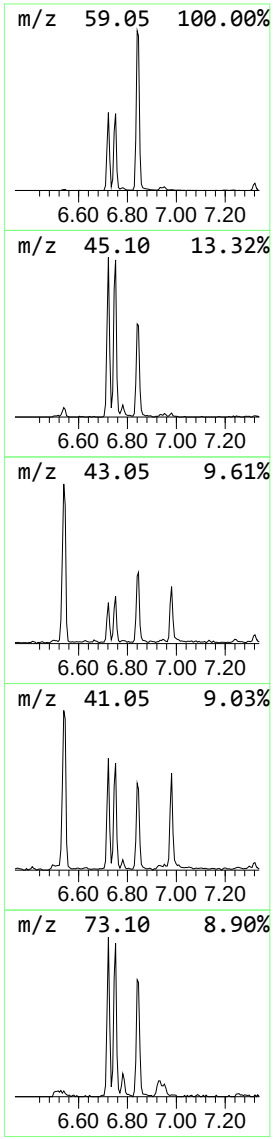
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Propanol, 1-(2-methoxypro... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.839	9.25 ng	304049	1,4-Dichlorobenzene-d4	6.928

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	83
2	2-Propanol, 1-(2-methoxypropoxy)-	148	C7H16O3	013429-07-7	78
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	78
4	Methane, diethoxy-	104	C5H12O2	000462-95-3	64
5	Tetraglyme	222	C10H22O5	000143-24-8	56





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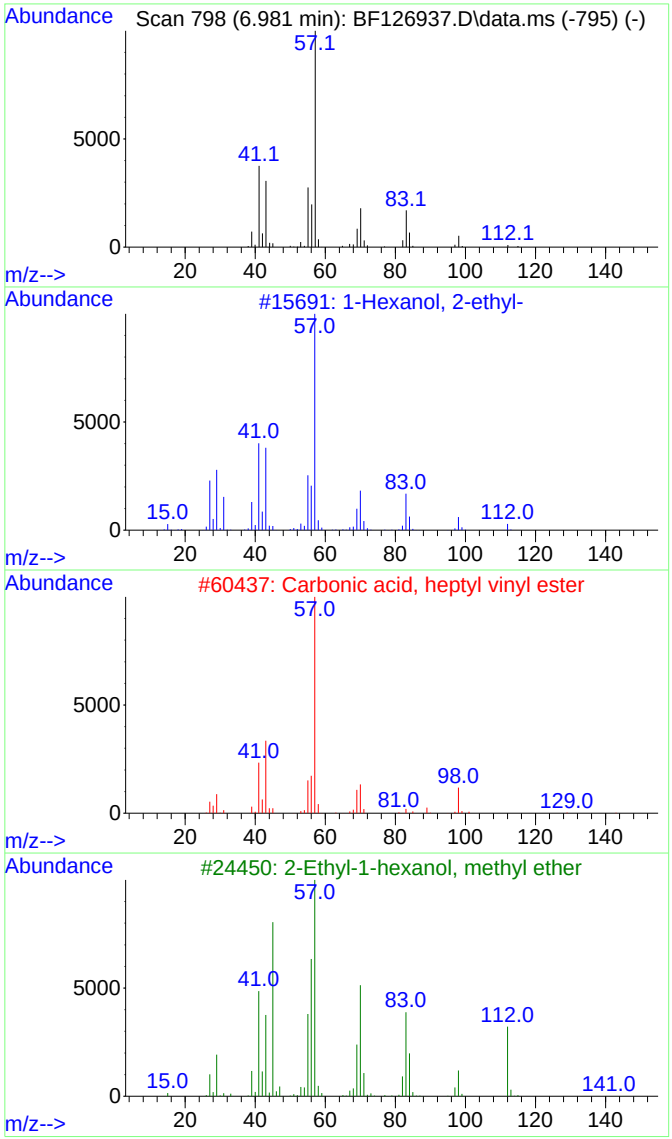
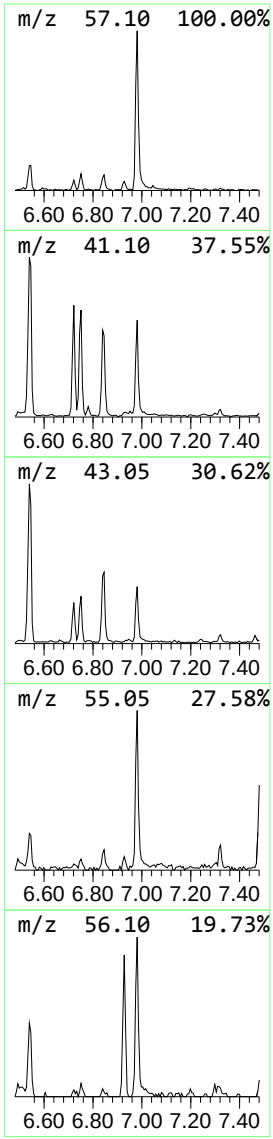
****

Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.981	3.95 ng	129648	1,4-Dichlorobenzene-d4	6.928

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	64
3	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	50
4	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
5	Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	45





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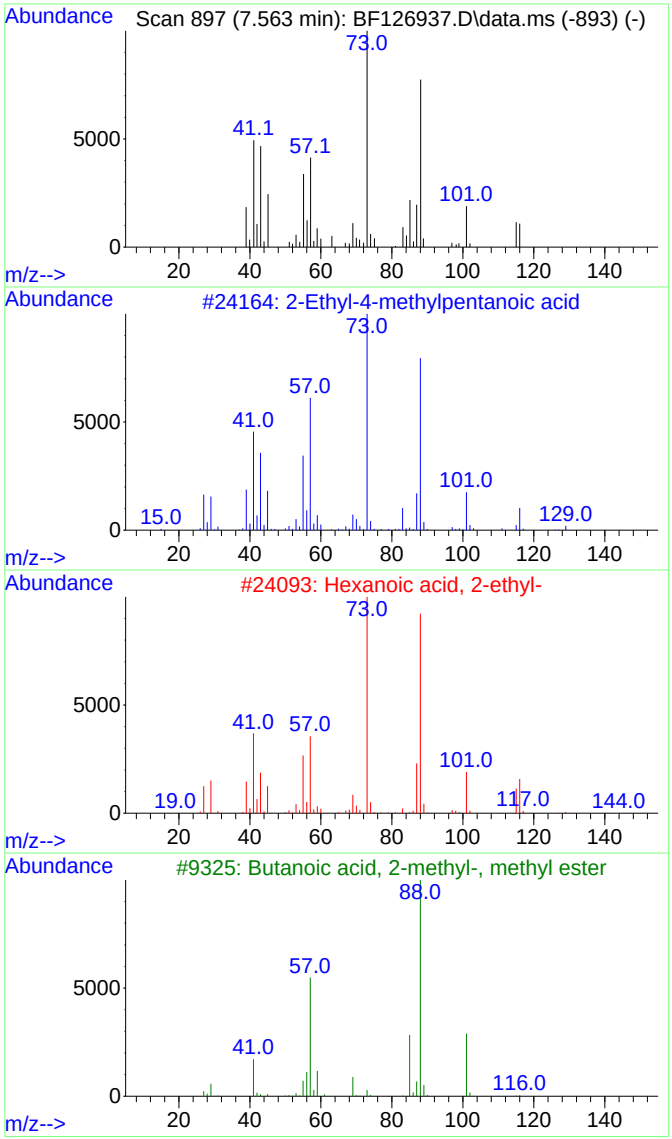
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

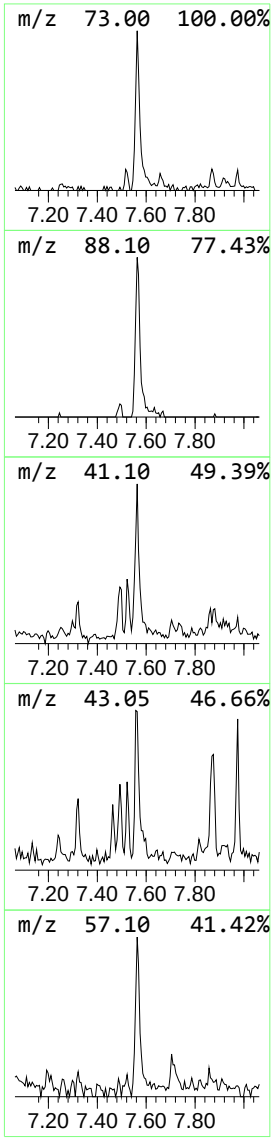
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 2-Ethyl-4-methylpentanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.563	2.14 ng	70309	1,4-Dichlorobenzene-d4	6.928

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	72
2	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	72
3	Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	47
4	Pentanoic acid, 2-methyl-, methy...	130	C7H14O2	002177-77-7	38
5	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	38





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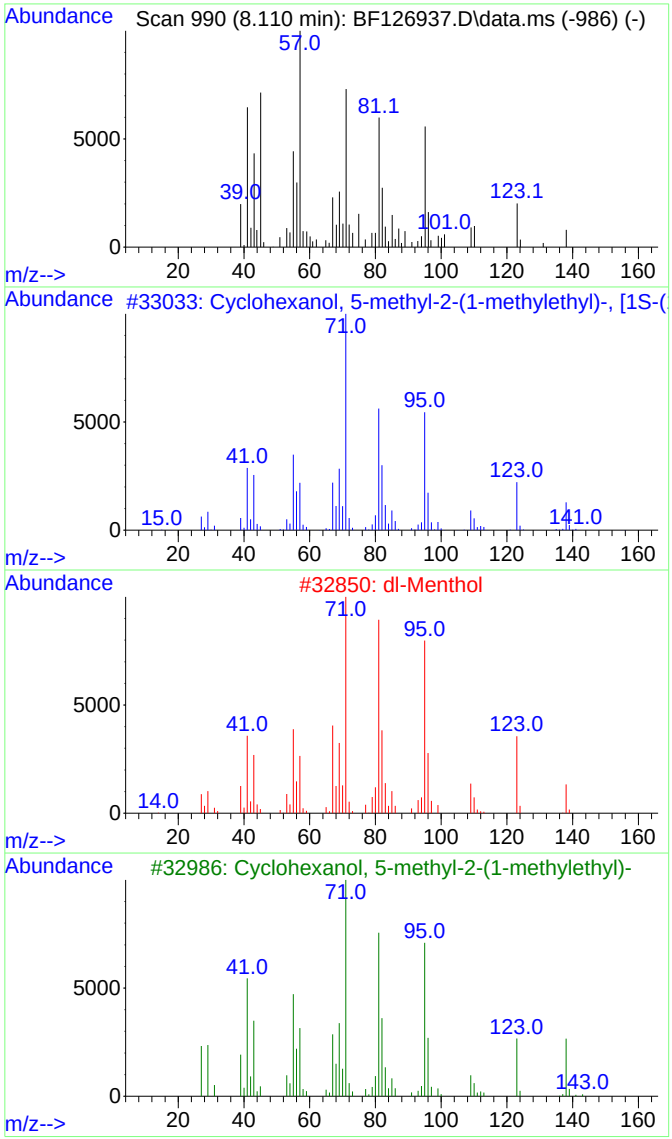
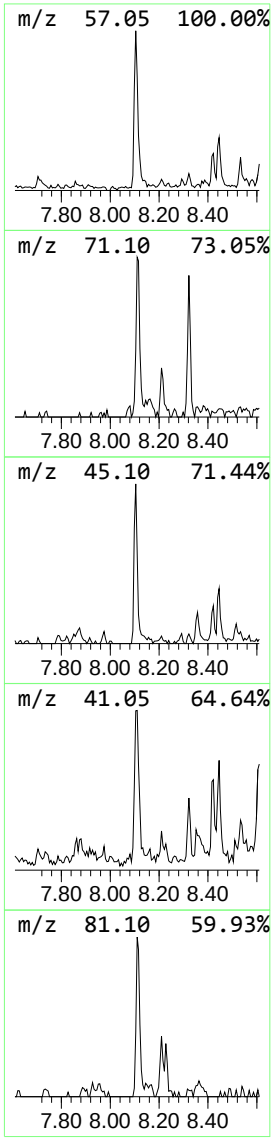
****
Peak Number 8 Cyclohexanol, 5-methyl-2-(1... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.110	2.41 ng	110292	Naphthalene-d8	8.210

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	023283-97-8	64
2	dl-Menthol	156	C10H20O	000089-78-1	62
3	Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	001490-04-6	58
4	Cyclohexanol, 1-methyl-4-(1-meth...	156	C10H20O	021129-27-1	58
5	Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	000491-02-1	58





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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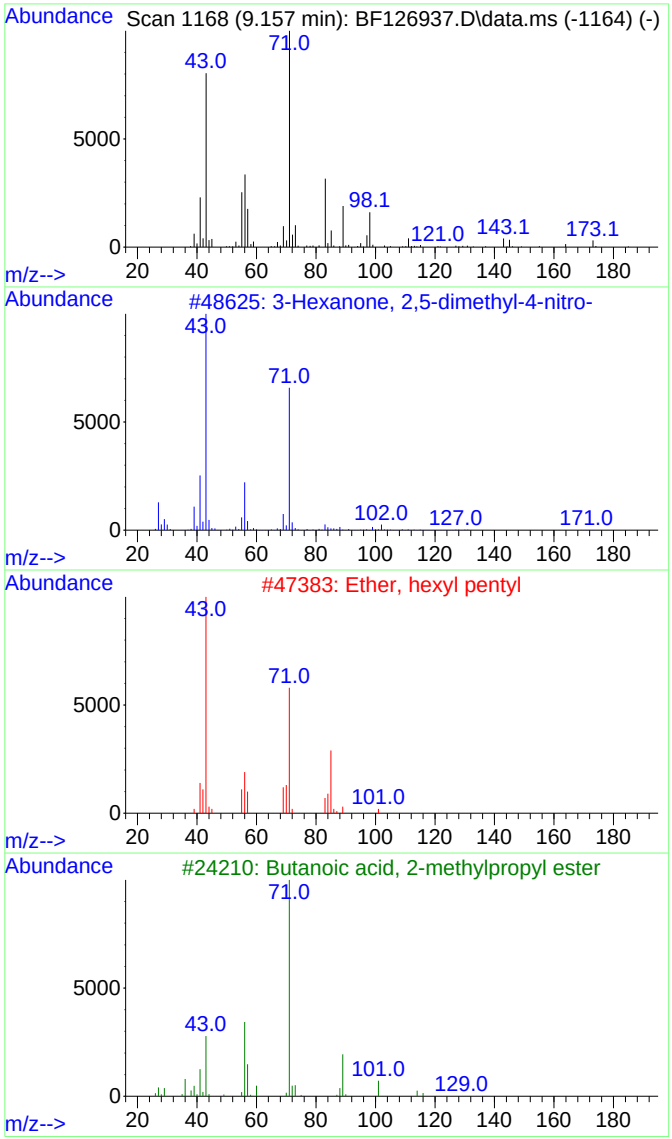
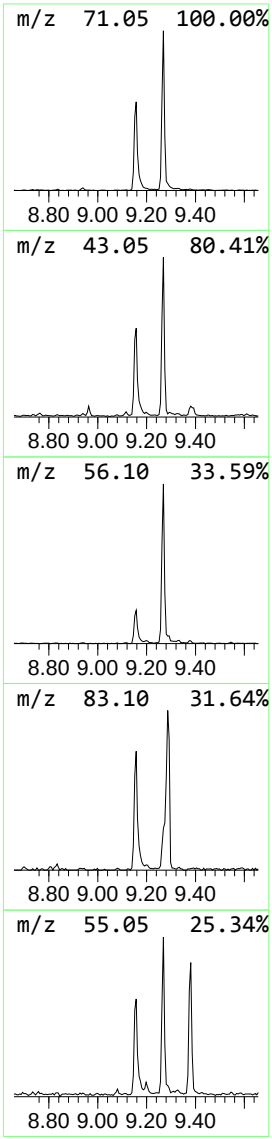
Peak Number 9 unknown9.157 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.157	5.51 ng	267860	Acenaphthene-d10	9.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexanone, 2,5-dimethyl-4-nitro-	173	C8H15NO3	059906-54-6	43
2	Ether, hexyl pentyl	172	C11H24O	032357-83-8	43
3	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	42
4	Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	40
5	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
Data File : BF126937.D
Acq On : 17 Feb 2022 20:14
Operator : CG\JU
Sample : N1573-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-20R

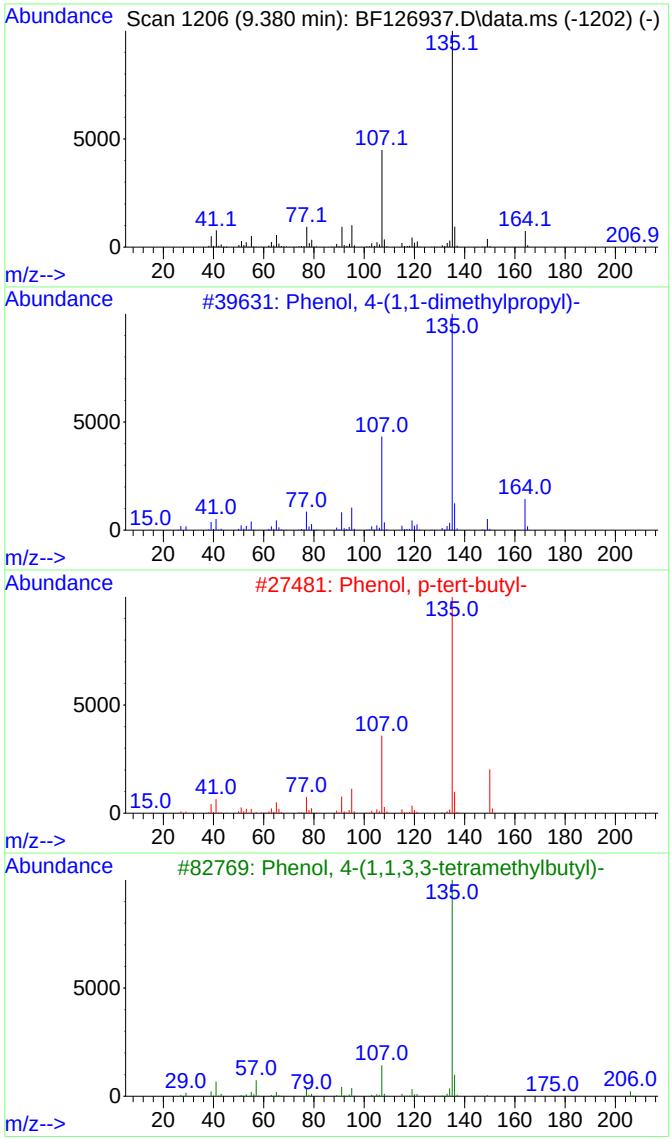
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

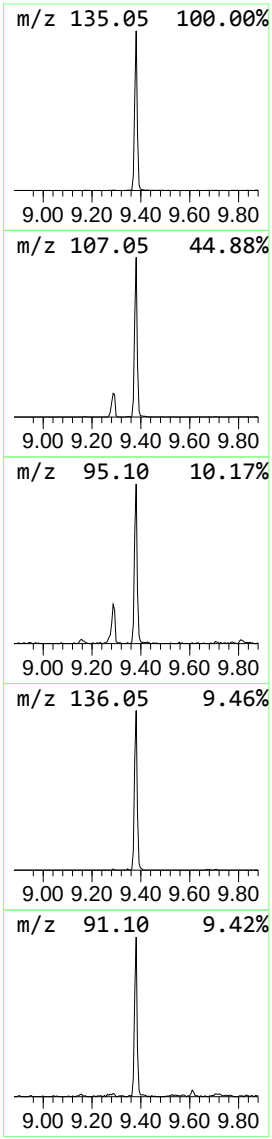
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Phenol, 4-(1,1-dimethylprop... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.380	17.09 ng	830171	Acenaphthene-d10	9.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	93
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	90
3	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	64
4	Hexestrol	270	C18H22O2	000084-16-2	64
5	4,4'-(1,2-diethylethylene)diphenol	270	C18H22O2	005635-50-7	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
Data File : BF126937.D
Acq On : 17 Feb 2022 20:14
Operator : CG\JU
Sample : N1573-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-20R

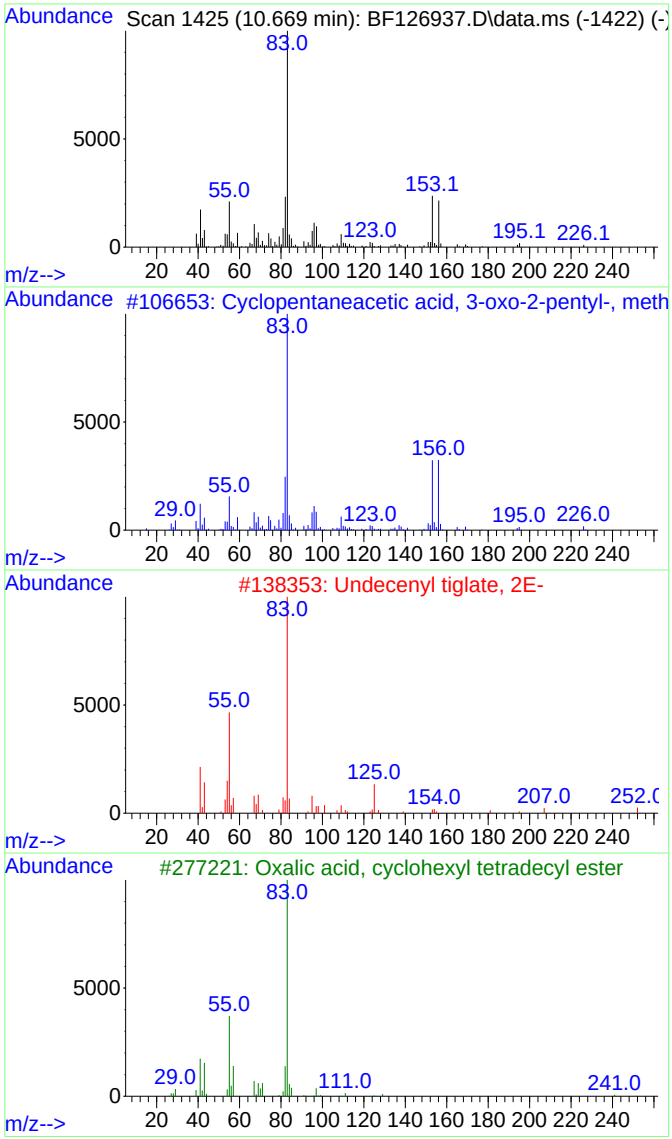
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

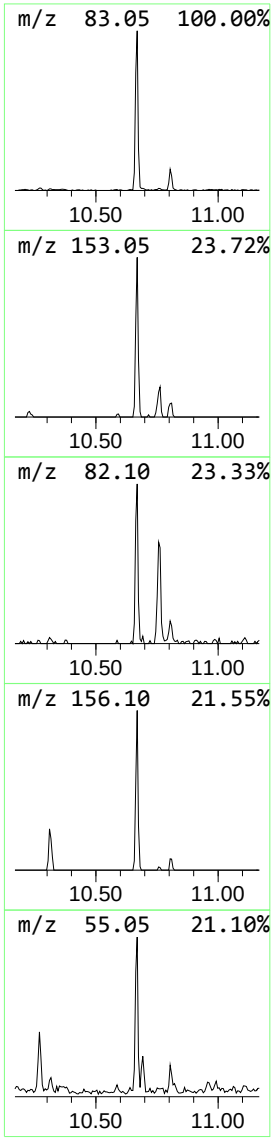
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Cyclopentaneacetic acid, 3-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.669	3.48 ng	169265	Acenaphthene-d10	9.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentaneacetic acid, 3-oxo-2...	226	C13H22O3	024851-98-7	93
2	Undecenyl tiglate, 2E-	252	C16H28O2	1000383-56-5	43
3	Oxalic acid, cyclohexyl tetradec...	368	C22H40O4	1000309-31-5	43
4	6-Hydroxy-10a-methyl-4,7-dimethy...	376	C20H24O7	1798297-60-5	38
5	Cyclohexane, 1,1'-(1,3-propanedi...	208	C15H28	003178-24-3	38





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Data File : BF126937.D
Acq On : 17 Feb 2022 20:14
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Sample : N1573-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-20R

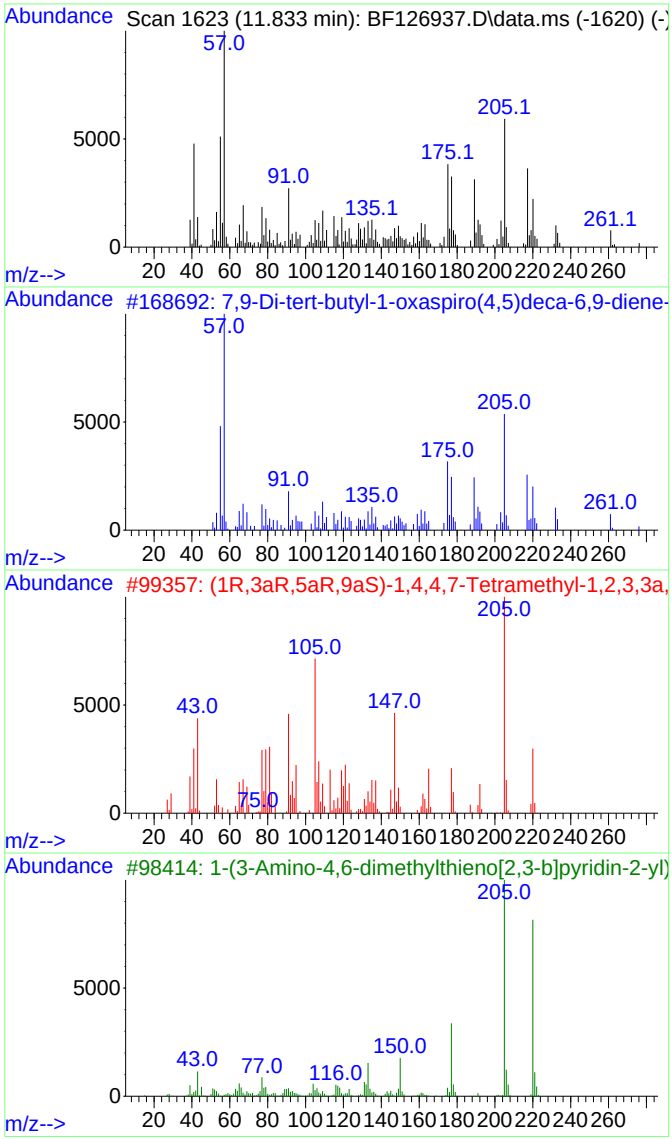
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

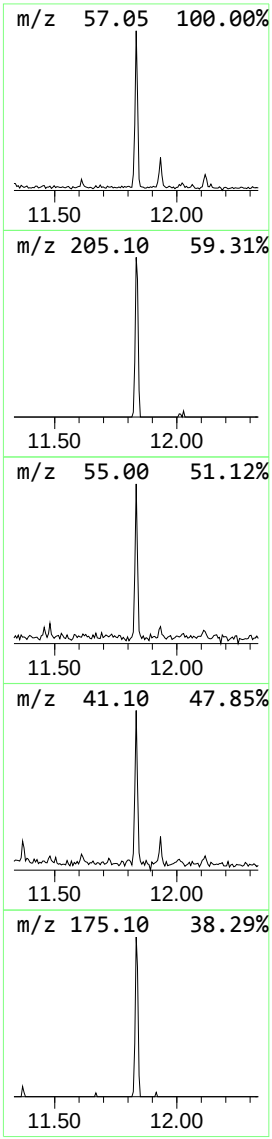
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.833	2.95 ng	151337	Phenanthrene-d10	11.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	99
2	(1R,3aR,5aR,9aS)-1,4,4,7-Tetrame...	220	C15H24O	104188-25-2	60
3	1-(3-Amino-4,6-dimethylthieno[2,...	220	C11H12N2OS	052505-42-7	46
4	1,3-Pentadiene, 1,1-diphenyl-, (Z)-	220	C17H16	015295-31-5	42
5	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
Data File : BF126937.D
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Misc :
ALS Vial : 17 Sample Multiplier: 1

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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.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
Cyclopentanone	4.457	12.6	ng	412432	1	6.928	657163	20.0
Ethanol, 2-(1-m...	5.157	4.7	ng	154679	1	6.928	657163	20.0
2-Propanol, 1-(...	6.722	5.4	ng	176812	1	6.928	657163	20.0
Dipropylene gly...	6.751	5.8	ng	189829	1	6.928	657163	20.0
2-Propanol, 1-(...	6.839	9.3	ng	304049	1	6.928	657163	20.0
1-Hexanol, 2-et...	6.981	4.0	ng	129648	1	6.928	657163	20.0
2-Ethyl-4-methy...	7.563	2.1	ng	70309	1	6.928	657163	20.0
Cyclohexanol, 5...	8.110	2.4	ng	110292	2	8.210	916274	20.0
unknown9.157	9.157	5.5	ng	267860	3	9.969	971421	20.0
Phenol, 4-(1,1-...	9.380	17.1	ng	830171	3	9.969	971421	20.0
Cyclopentaneace...	10.669	3.5	ng	169265	3	9.969	971421	20.0
7,9-Di-tert-but...	11.833	3.0	ng	151337	4	11.457	1026990	20.0