LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
Data File : BF126930.D
Acq On : 17 Feb 2022 16:49
Operator : CG\JU
Sample : N1573-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-23R

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: BF126930.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.469	366	371	377	rVB	393380	448428	8.85%	1.610%
2	5.163	485	489	495	rVB	128901	141918	2.80%	0.510%
3	5.551	550	555	558	rBV	2228487	2064363	40.75%	7.412%
4	6.545	719	724	727	rVB	1675660	1521614	30.04%	5.463%
5	6.722	751	754	756	rBV	263845	191655	3.78%	0.688%
6	6.751	756	759	762	rVB	266079	202940	4.01%	0.729%
7	6.845	771	775	778	rBV	370563	330376	6.52%	1.186%
8	6.928	785	789	792	rBV	803262	607158	11.99%	2.180%
9	6.981	795	798	809	rVB	761821	630935	12.46%	2.265%
10	7.104	817	819	822	rVB	103109	87377	1.72%	0.314%
11	7.492	880	885	888	rVB	2577032	2744309	54.18%	9.854%
12	7.575	893	899	906	rBV2	117946	190153	3.75%	0.683%
13	8.110	986	990	994	rBV3	64247	90907	1.79%	0.326%
14	8.210	1003	1007	1010	rBV	1012276	833700	16.46%	2.993%
15	8.357	1030	1032	1040	rBV	58124	66222	1.31%	0.238%
16	8.539	1056	1063	1068	rBV3	89756	134955	2.66%	0.485%
17	8.928	1126	1129	1134	rBV2	57544	56120	1.11%	0.202%
18	9.157	1164	1168	1173	rBV	217301	239569	4.73%	0.860%
19	9.292	1184	1191	1193	rBV	4607519	4876018	96.26%	17.507%
20	9.380	1202	1206	1209	rBV	1038256	792804	15.65%	2.847%
21	9.710	1258	1262	1267	rVB4	41832	60260	1.19%	0.216%
22	9.969	1303	1306	1309	rVB	1143636	877415	17.32%	3.150%
23	10.380	1372	1376	1380	rVB	177084	149757	2.96%	0.538%
24	10.669	1422	1425	1427	rBV	166060	121169	2.39%	0.435%
25	10.763	1436	1441	1444	rBV	3428971	3147846	62.14%	11.302%
26	11.457	1555	1559	1563	rBV	1151664	934111	18.44%	3.354%
27	11.833	1620	1623	1626	rBV	168388	130444	2.58%	0.468%
28	13.051	1824	1830	1833	rBV	5176381	5065587	100.00%	18.188%
29	14.098	2005	2008	2012	rBV	680020	590133	11.65%	2.119%
30	15.604	2258	2264	2273	rVB	420742	522804	10.32%	1.877%

Sum of corrected areas: 27851047

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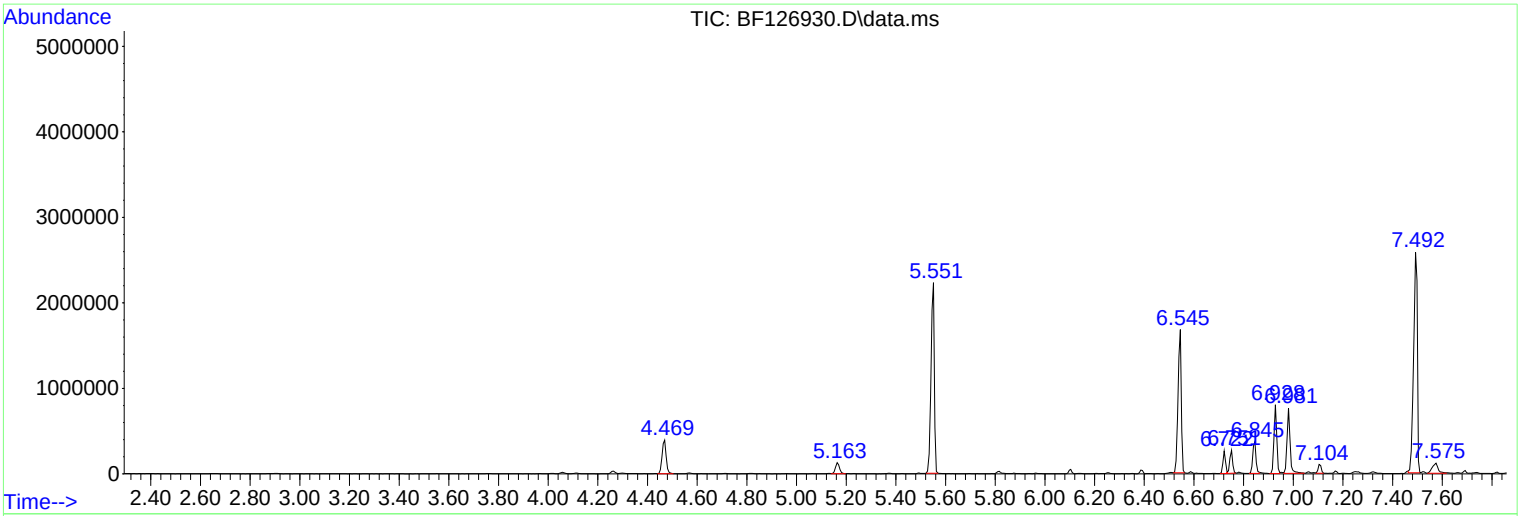
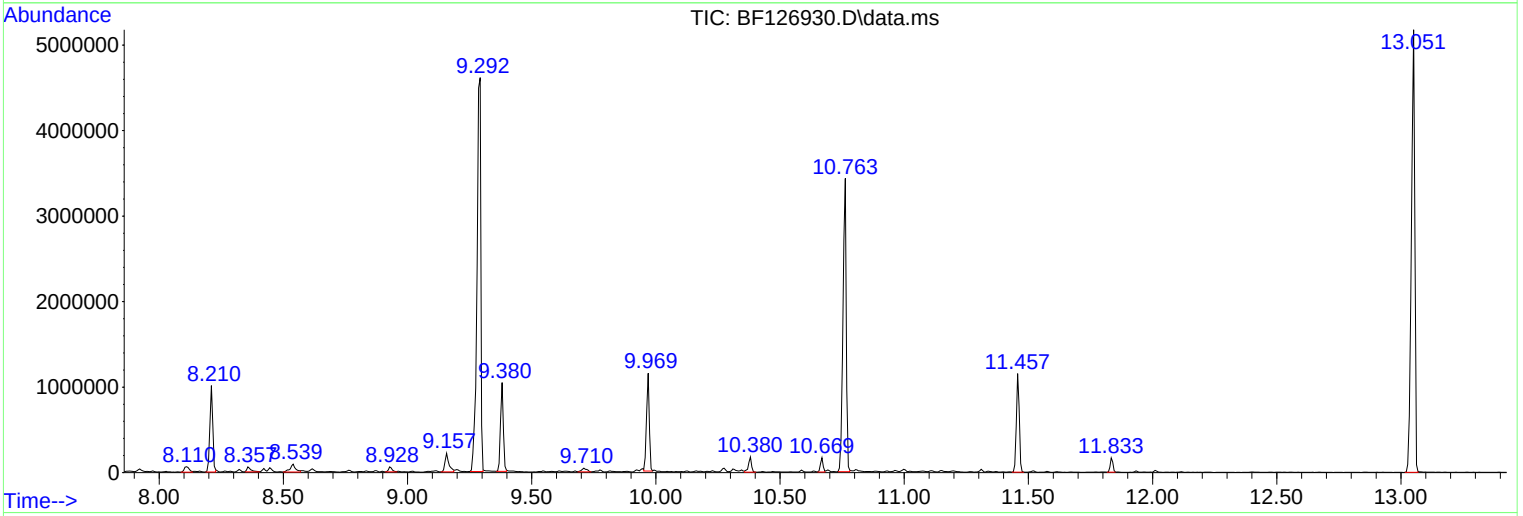
Acq On : 17 Feb 2022 16:49
Operator : CG\JU
Sample : N1573-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

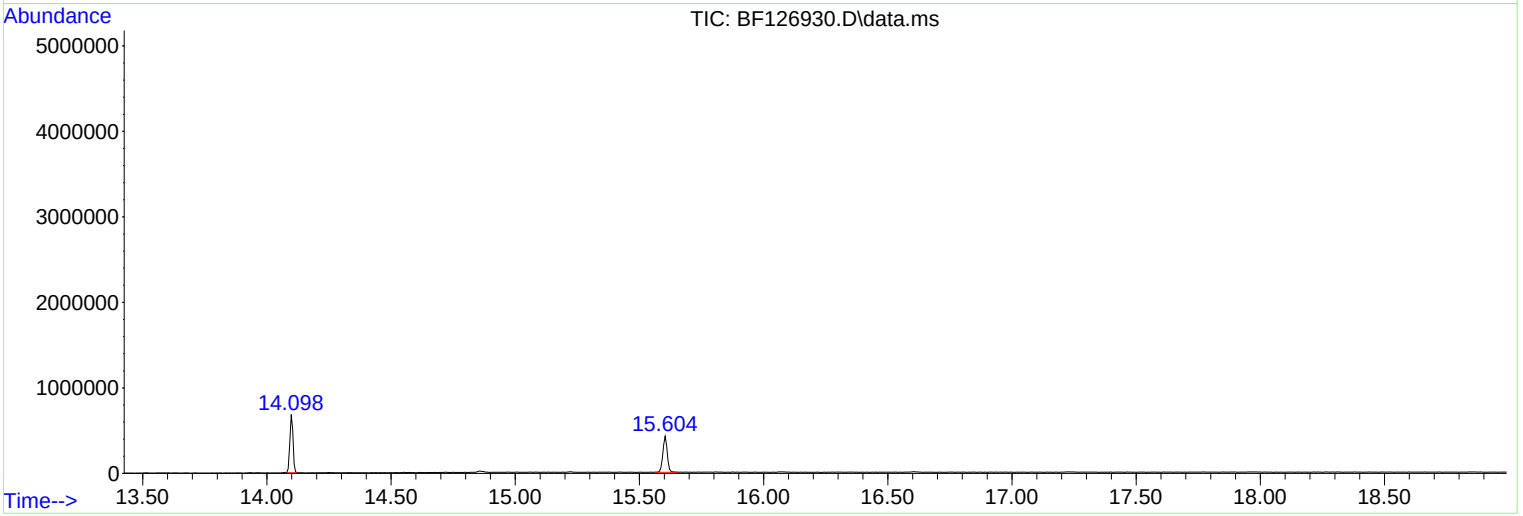
Instrument :
BNA_F
ClientSampleId :
MW-23R

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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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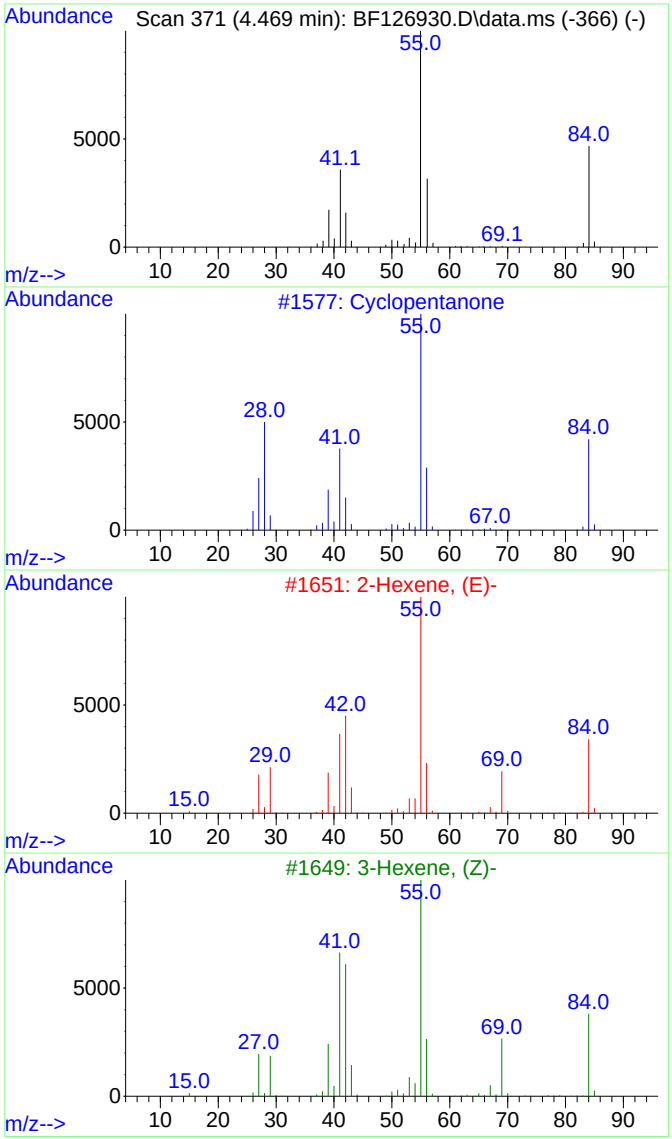
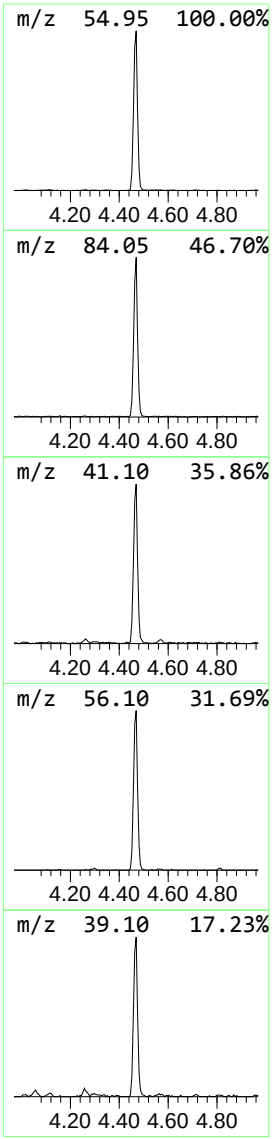
****

Peak Number 1 Cyclopentanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.469	14.77 ng	448428	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	64
3	3-Hexene, (Z)-	84	C6H12	007642-09-3	59
4	2(5H)-Furanone	84	C4H4O2	000497-23-4	50
5	2-Hexene	84	C6H12	000592-43-8	50





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Misc :
ALS Vial : 10 Sample Multiplier: 1

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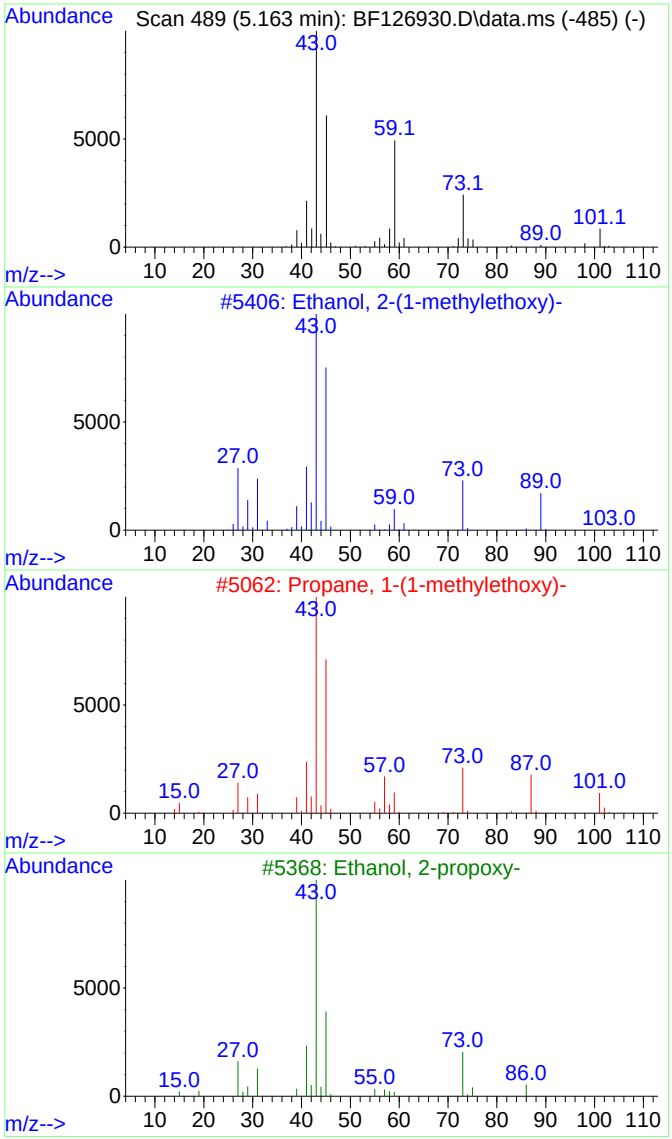
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

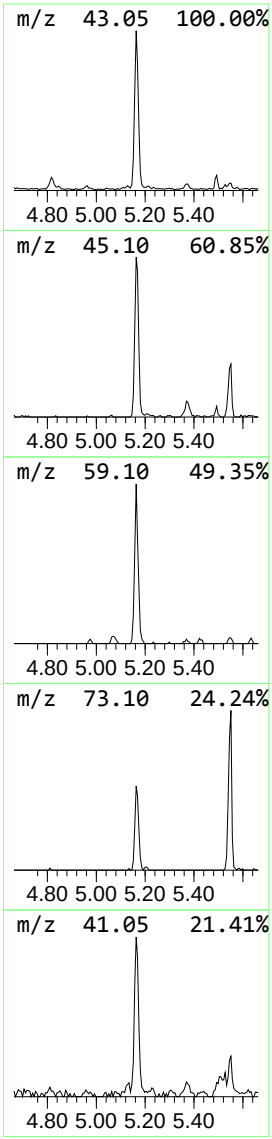
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol, 2-(1-methylethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.163	4.67 ng	141918	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	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	47
3	Ethanol, 2-propoxy-	104	C5H12O2	002807-30-9	43
4	Butane, 1-(1-methylethoxy)-	116	C7H16O	001860-27-1	38
5	Butanoic acid, 4-methoxy-	118	C5H10O3	029006-02-8	38





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Misc :
ALS Vial : 10 Sample Multiplier: 1

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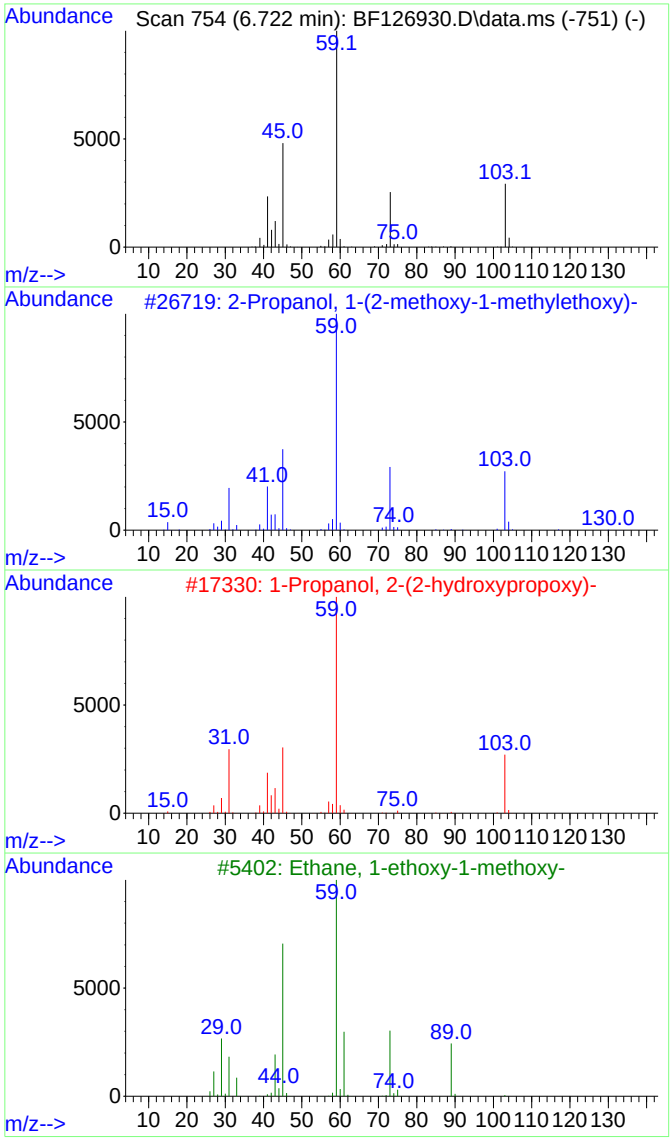
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

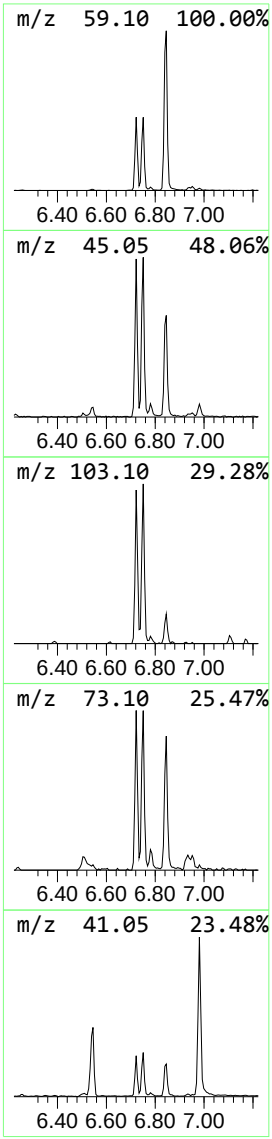
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.722	6.31 ng	191655	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	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	53
3	Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	50
4	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	50
5	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	50





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Operator : CG\JU
Sample : N1573-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-23R

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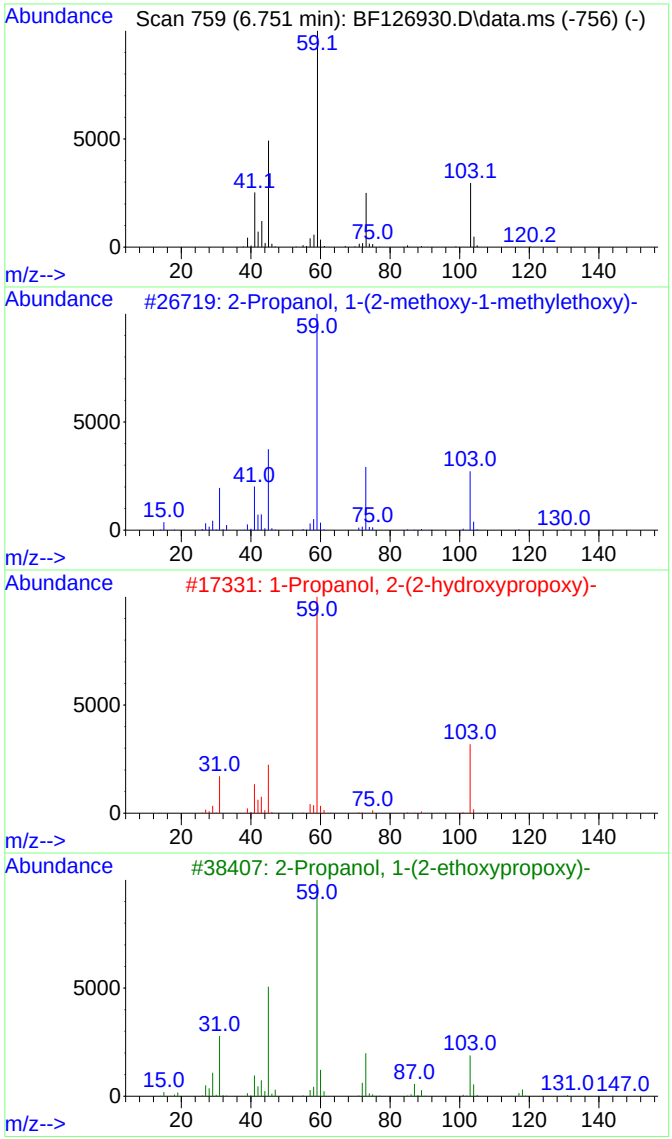
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

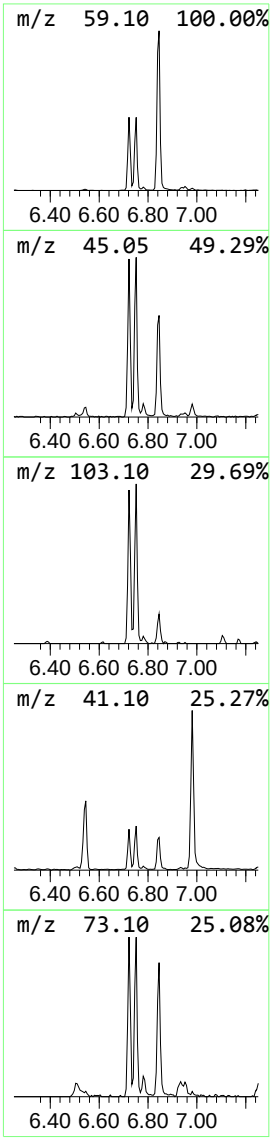
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Propanol, 2-(2-hydroxypro... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.751	6.68 ng	202940	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	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	59
3	2-Propanol, 1-(2-ethoxypropoxy)-	162	C8H18O3	010143-32-5	56
4	2-Propanol, 1,1'-[(1-methyl-1,2-...	192	C9H20O4	001638-16-0	53
5	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	50





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Sample : N1573-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-23R

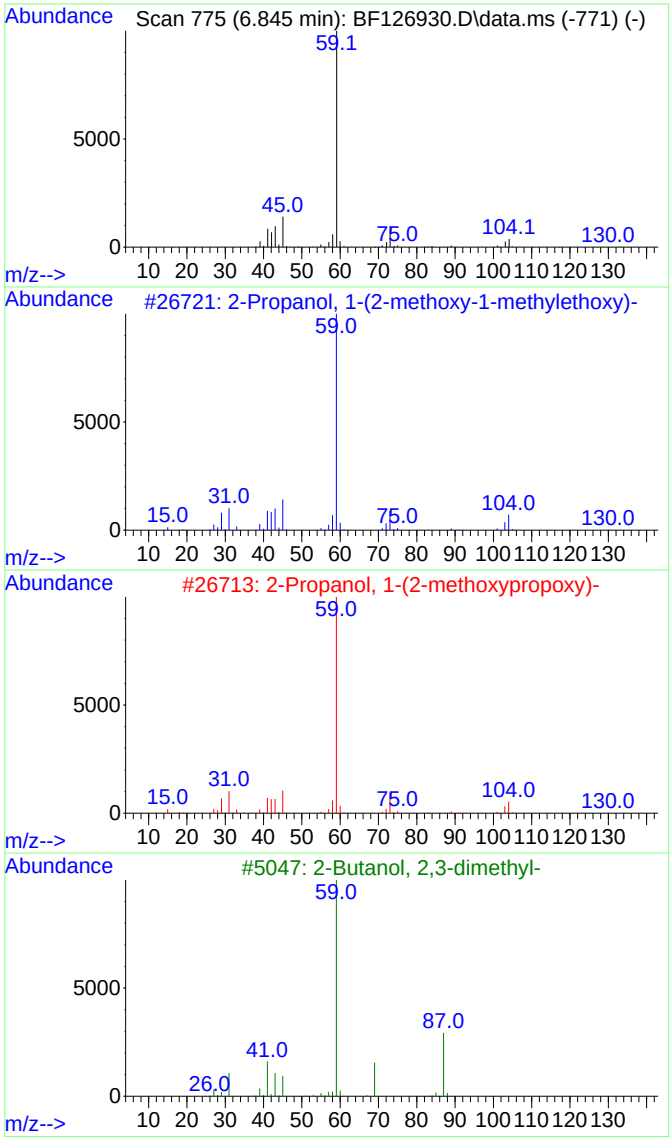
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

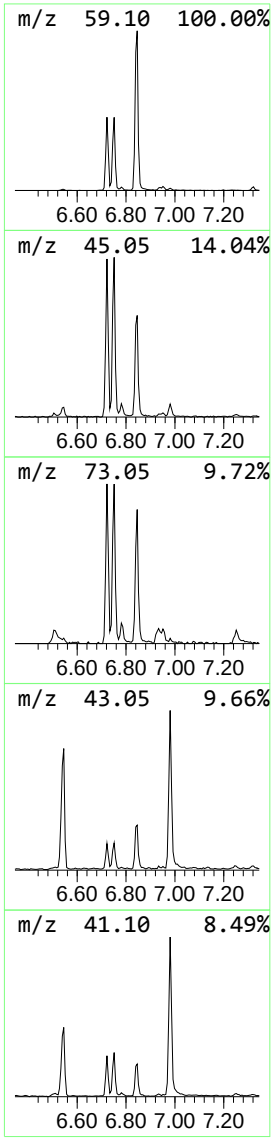
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Propanol, 1-(2-methoxypro... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.845	10.88 ng	330376	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	83
3	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	45
4	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	43
5	1-(1-Methoxypropan-2-yloxy)propa...	190	C9H18O4	1000367-08-6	40





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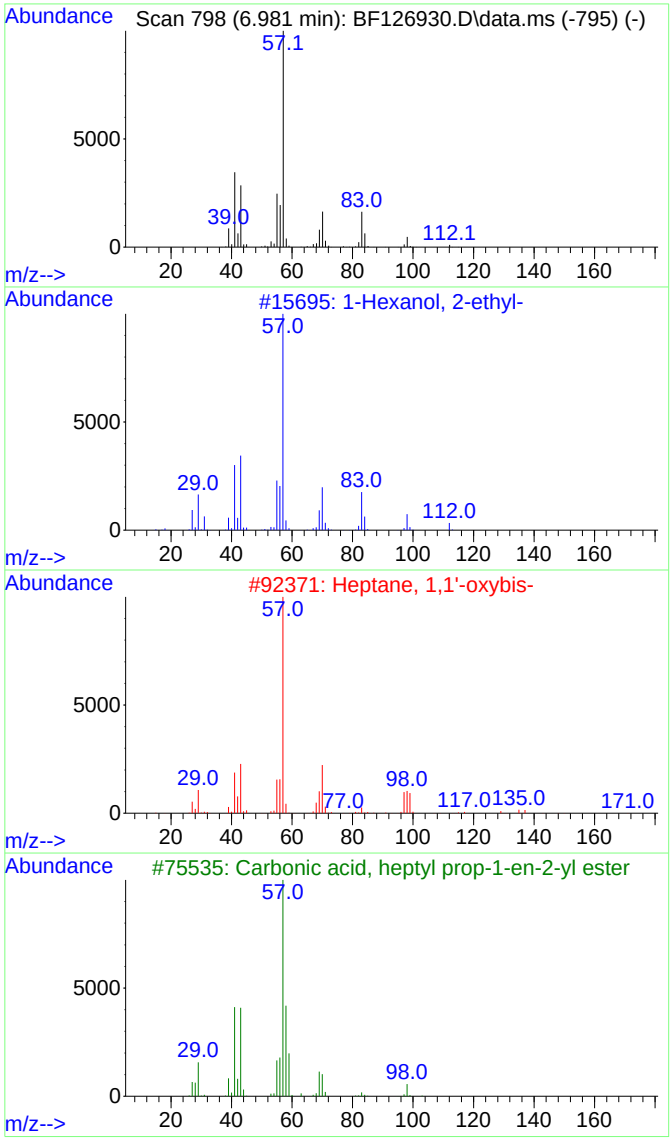
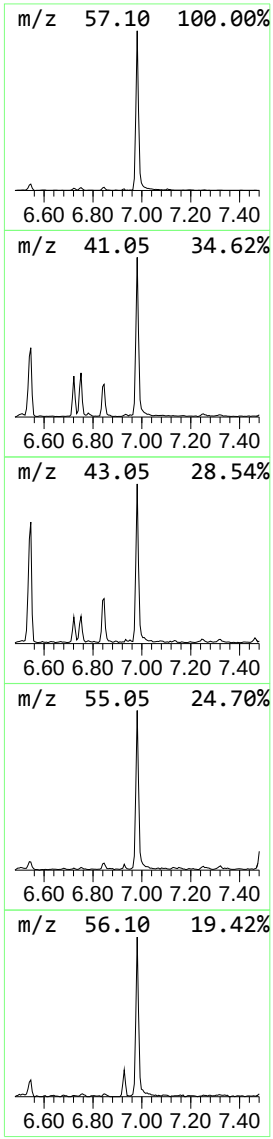
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.981	20.78 ng	630935	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	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
3	Carbonic acid, heptyl prop-1-en-...	200	C11H20O3	1000382-54-1	43
4	Oxalic acid, isobutyl heptyl ester	244	C13H24O4	1000309-37-2	42
5	Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	42





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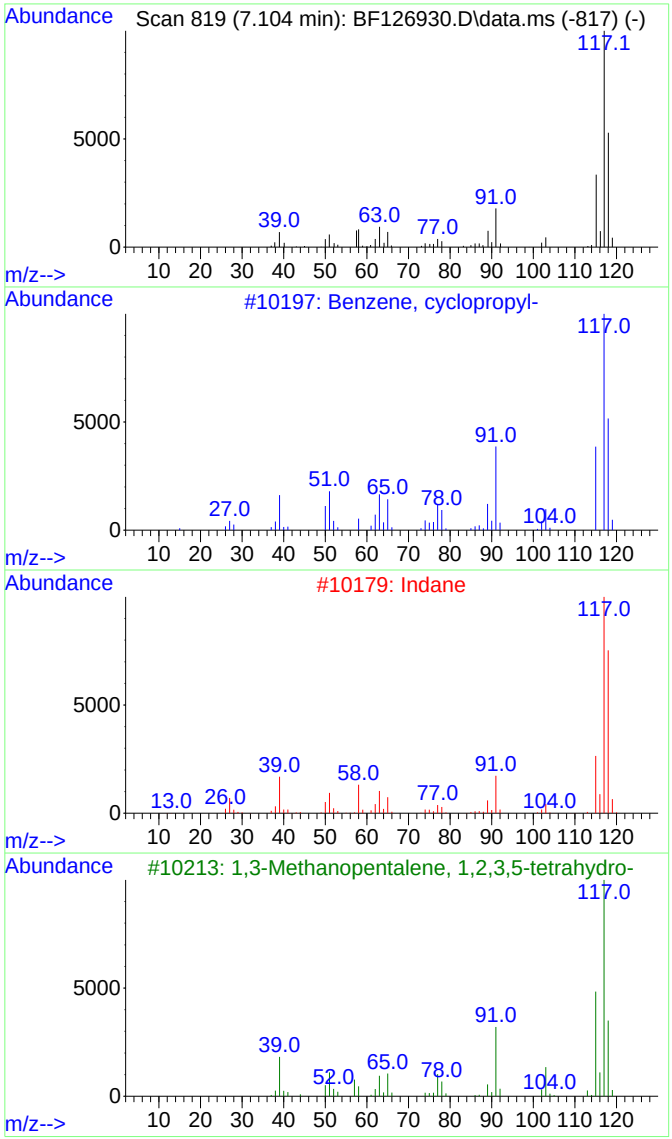
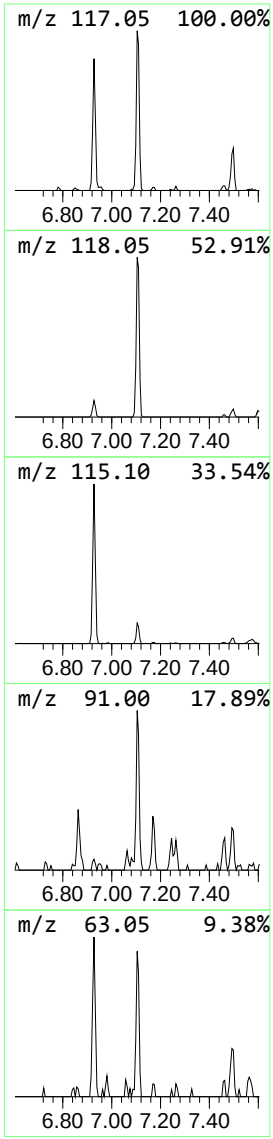
****

Peak Number 7 Benzene, cyclopropyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.104	2.88 ng	87377	1,4-Dichlorobenzene-d4	6.928

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, cyclopropyl-	118	C9H10	000873-49-4	94
2	Indane	118	C9H10	000496-11-7	93
3	1,3-Methanopentalene, 1,2,3,5-te...	118	C9H10	128600-88-4	72
4	Deltacyclene	118	C9H10	007785-10-6	68
5	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	64





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TIC Library : C:\Database\NIST20.L
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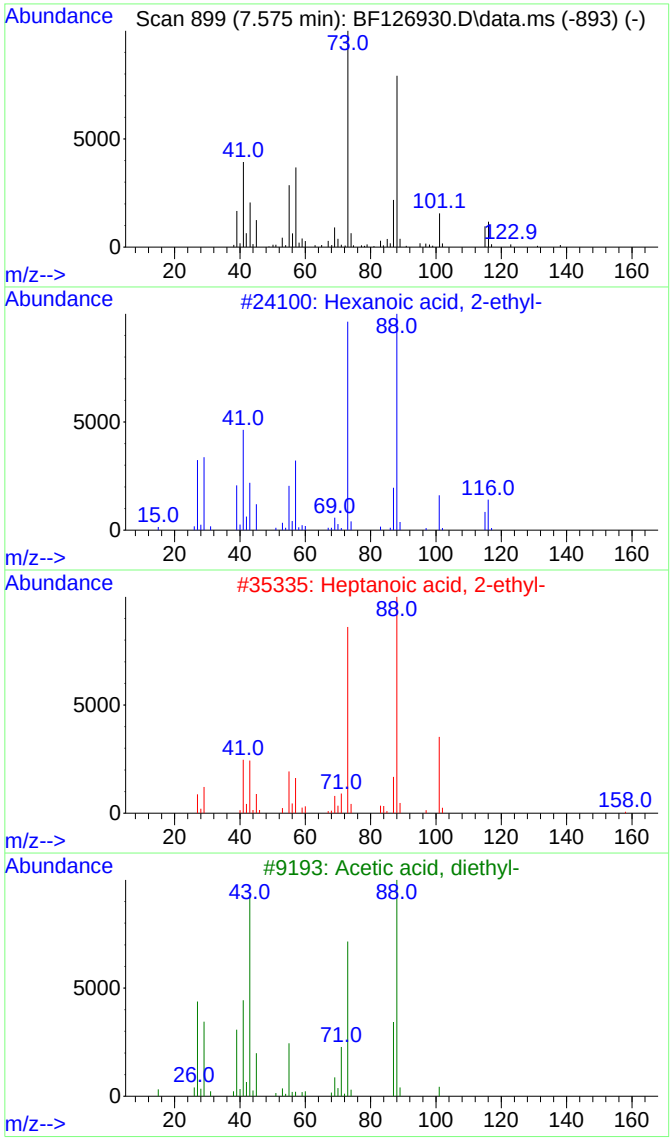
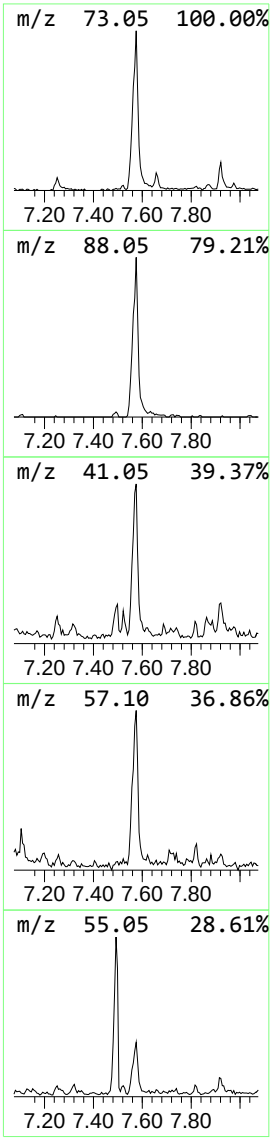
Peak Number 8 Hexanoic acid, 2-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.575	4.56 ng	190153	Naphthalene-d8	8.210

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	53
3	Acetic acid, diethyl-	116	C6H12O2	000088-09-5	45
4	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	45
5	1,4-Dioxane	88	C4H8O2	000123-91-1	43





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Instrument :
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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
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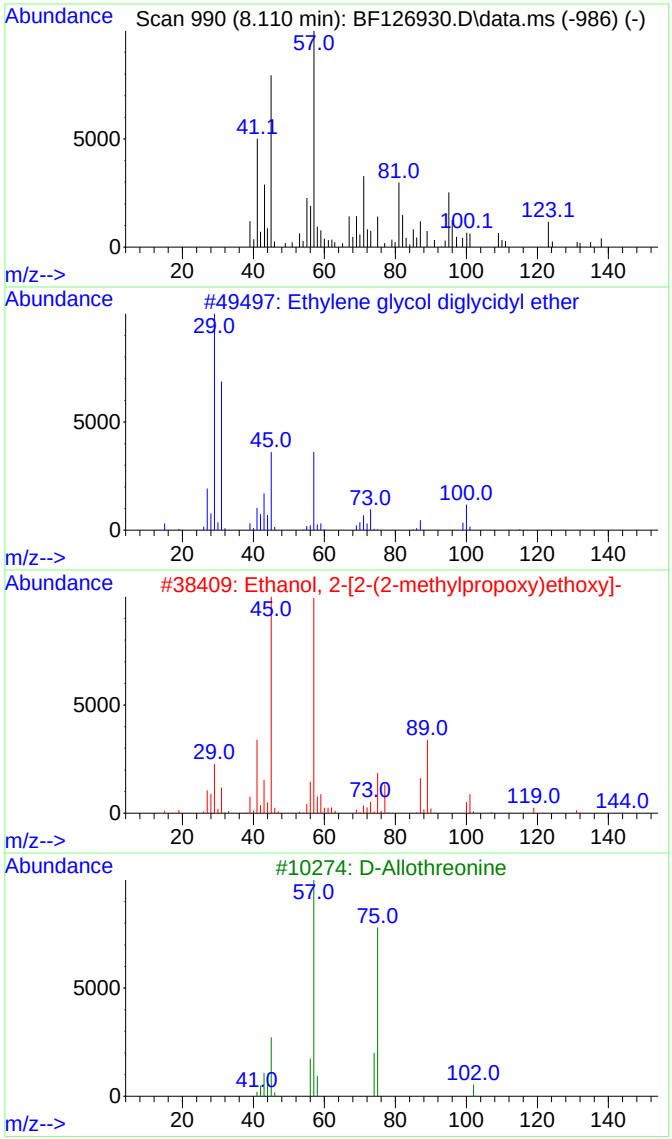
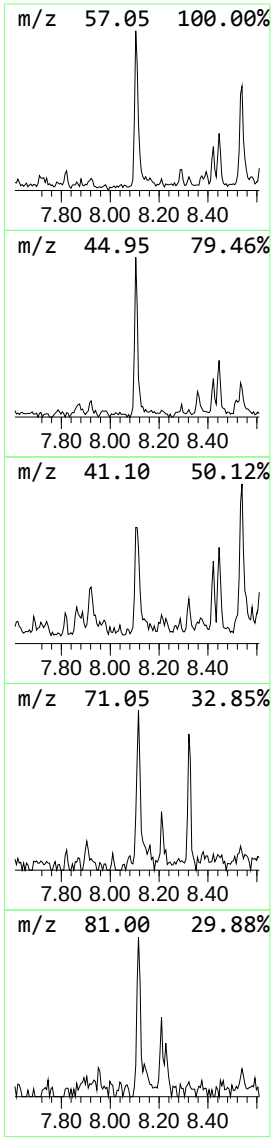
Peak Number 9 unknown8.110 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.110	2.18 ng	90907	Naphthalene-d8	8.210

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethylene glycol diglycidyl ether	174	C8H14O4	002224-15-9	47
2	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	47
3	D-Allothreonine	119	C4H9NO3	024830-94-2	47
4	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	46
5	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	46





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Data File : BF126930.D
Acq On : 17 Feb 2022 16:49
Operator : CG\JU
Sample : N1573-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-23R

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

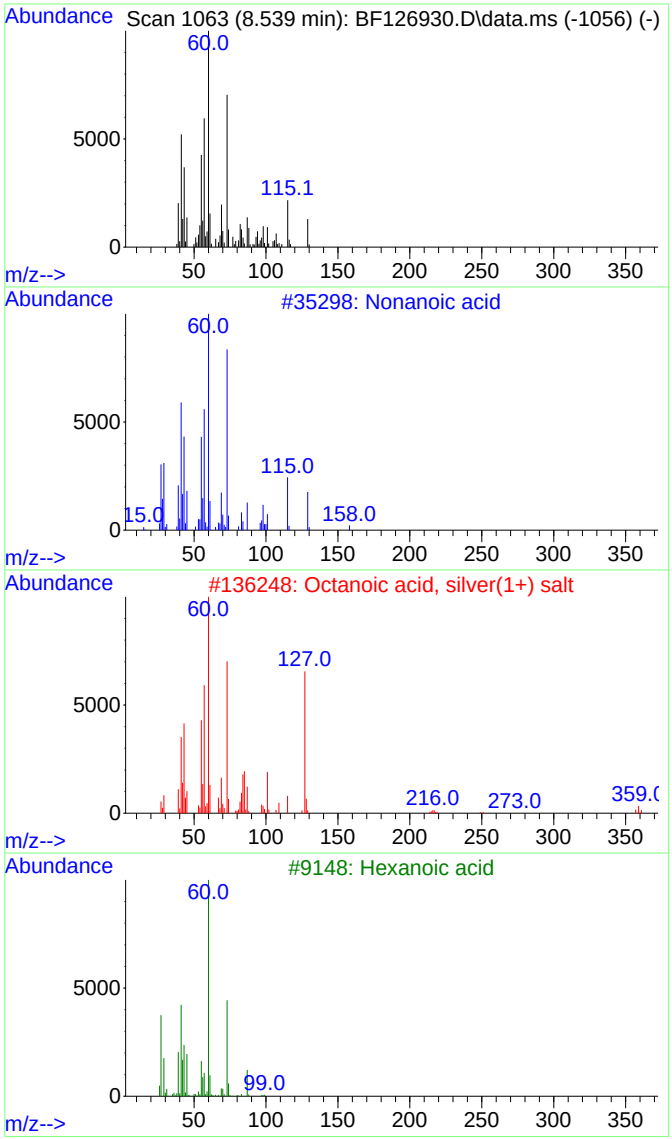
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

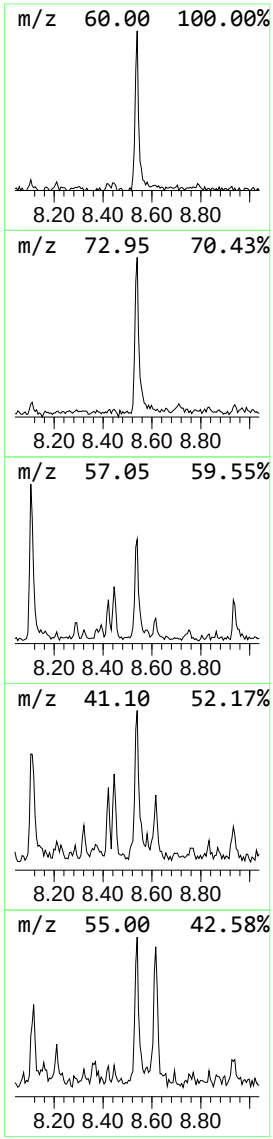
****

Peak Number 10 Nonanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.539	3.24 ng	134955	Naphthalene-d8	8.210

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanoic acid	158	C9H18O2	000112-05-0	90
2	Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	52
3	Hexanoic acid	116	C6H12O2	000142-62-1	50
4	Thiazole, 2-ethyl-4,5-dihydro-	115	C5H9NS	016982-46-0	50
5	Heptanoic acid	130	C7H14O2	000111-14-8	50





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Acq On : 17 Feb 2022 16:49
Operator : CG\JU
Sample : N1573-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-23R

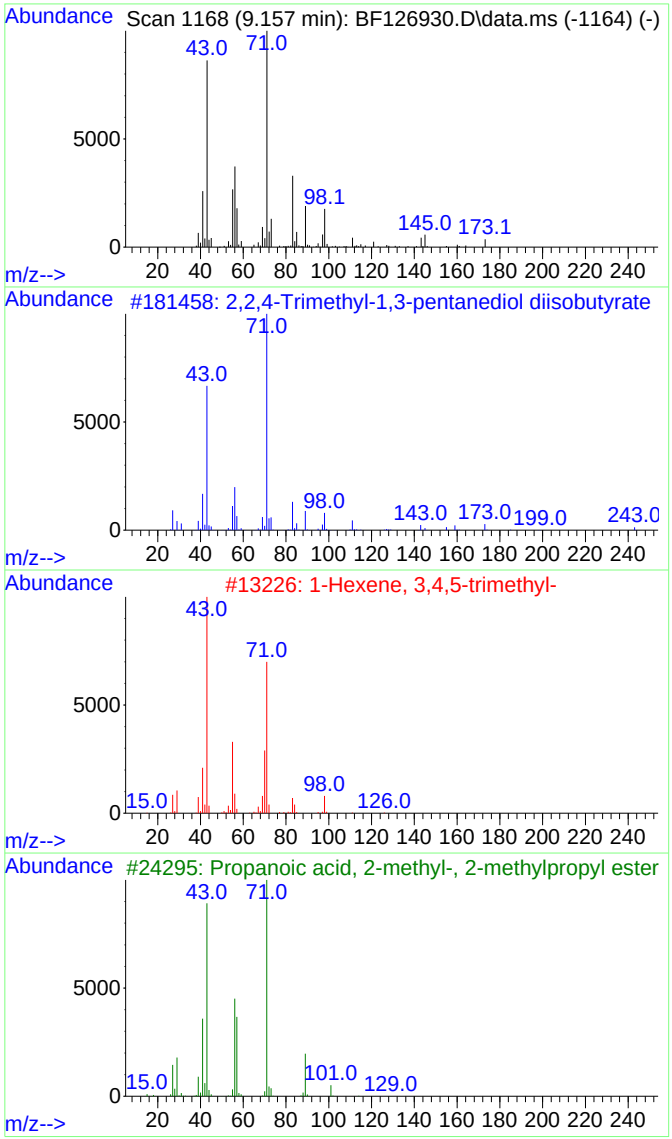
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

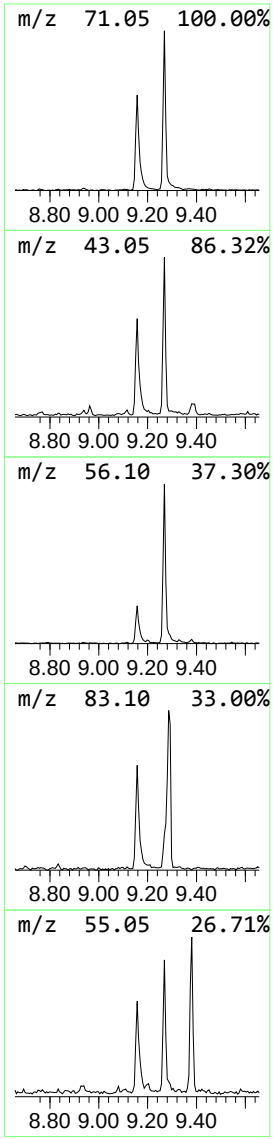
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 2,2,4-Trimethyl-1,3-pentane... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.157	5.46 ng	239569	Acenaphthene-d10	9.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	64
2	1-Hexene, 3,4,5-trimethyl-	126	C9H18	056728-10-0	43
3	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	40
4	Propanoic acid, 2-methyl-, 3-hyd...	216	C12H24O3	000077-68-9	38
5	Acrolein,dimethyl acetal	102	C5H10O2	006044-68-4	38





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Data File : BF126930.D
Acq On : 17 Feb 2022 16:49
Operator : CG\JU
Sample : N1573-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-23R

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

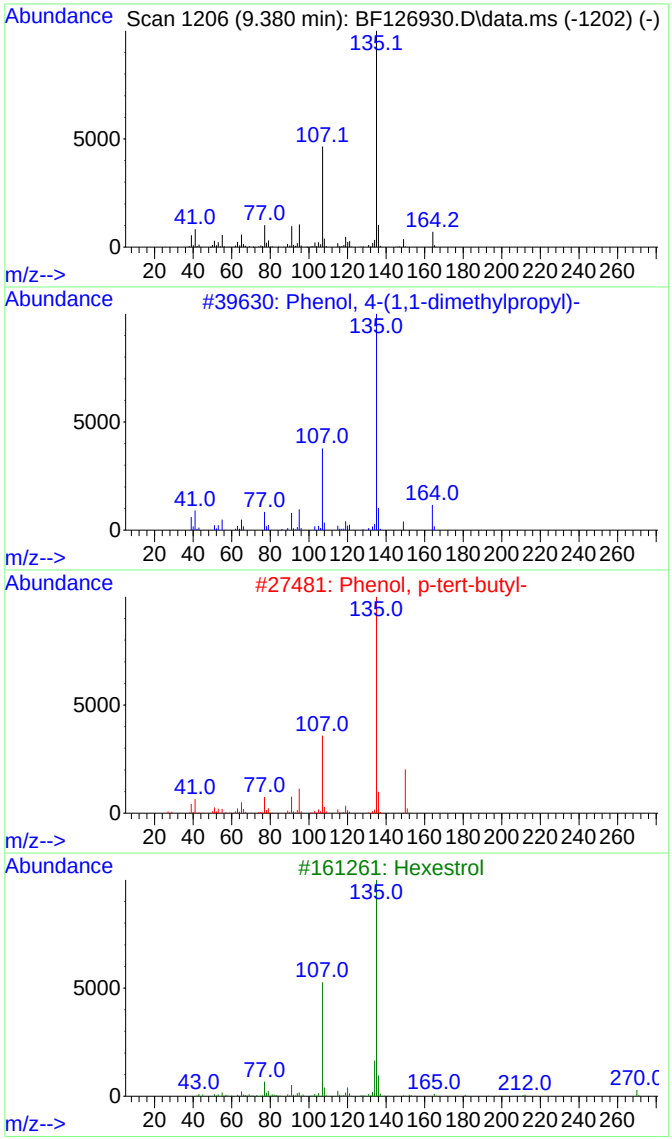
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

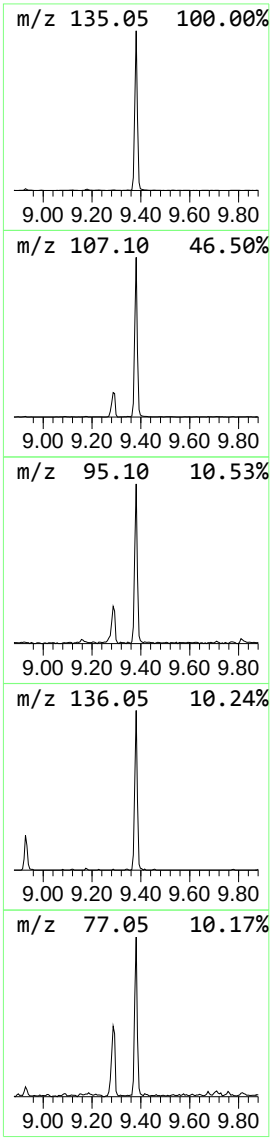
****

Peak Number 12 Phenol, 4-(1,1-dimethylprop... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.380	18.07 ng	792804	Acenaphthene-d10	9.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	91
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	90
3	Hexestrol	270	C18H22O2	000084-16-2	72
4	Hexestrol, O-trifluoroacetyl-	366	C20H21F3O3	1000365-31-7	72
5	4,4'-(1,2-diethylethylene)diphenol	270	C18H22O2	005635-50-7	64





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Data File : BF126930.D
Acq On : 17 Feb 2022 16:49
Operator : CG\JU
Sample : N1573-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-23R

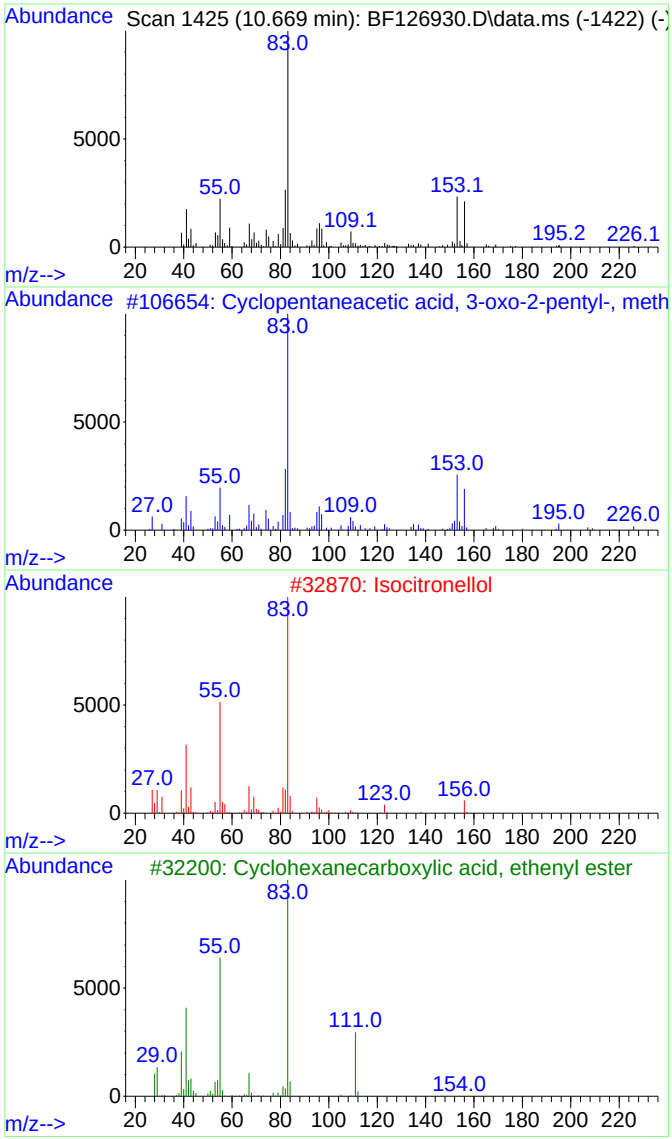
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

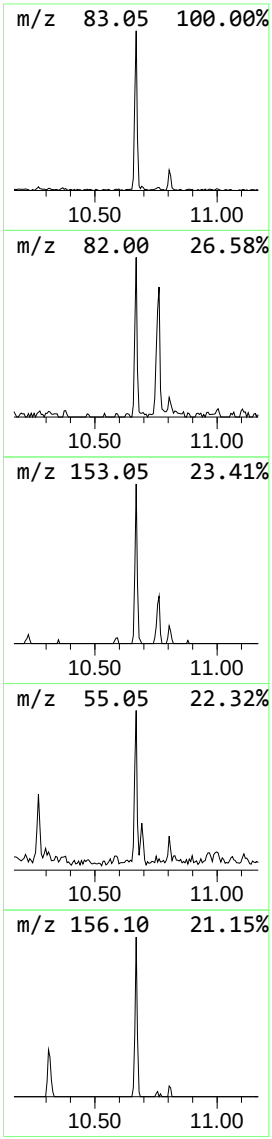
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 Cyclopentaneacetic acid, 3-... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.669	2.76 ng	121169	Acenaphthene-d10	9.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentaneacetic acid, 3-oxo-2...	226	C13H22O3	024851-98-7	90
2	Isocitronellol	156	C10H20O	018479-52-2	53
3	Cyclohexanecarboxylic acid, ethe...	154	C9H14O2	004840-76-0	43
4	N-(Piperidin-3-yl)acetamide	142	C7H14N2O	005810-55-9	43
5	Hexanal di-cis-3-hexenyl acetal	282	C18H34O2	1000430-94-7	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
Data File : BF126930.D
Acq On : 17 Feb 2022 16:49
Operator : CG\JU
Sample : N1573-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-23R

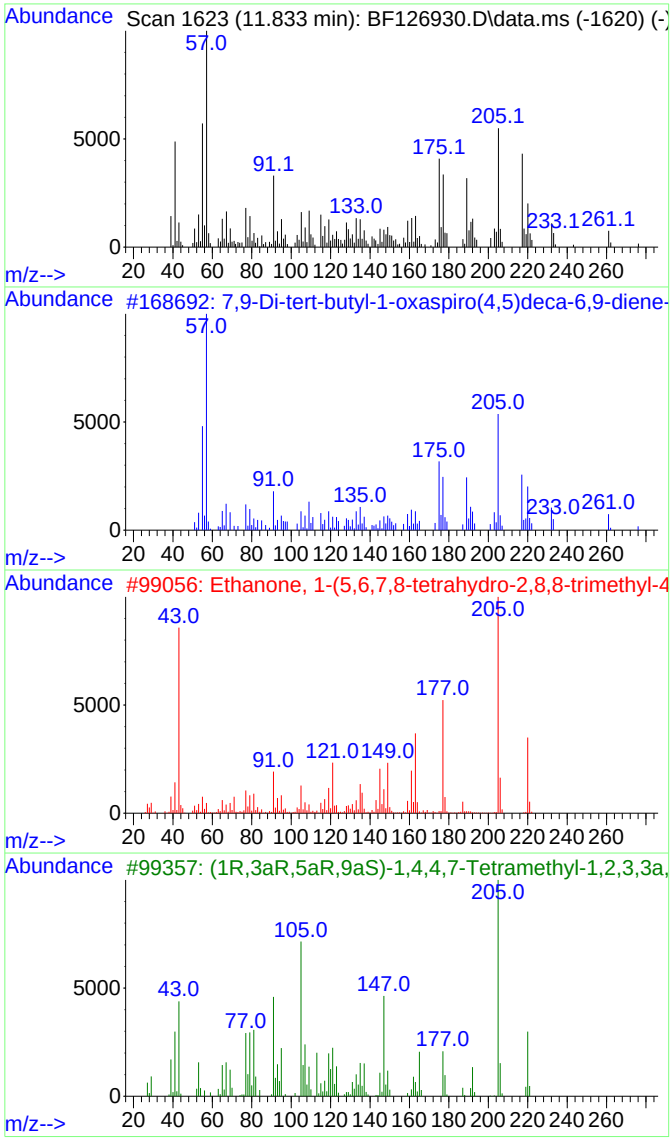
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

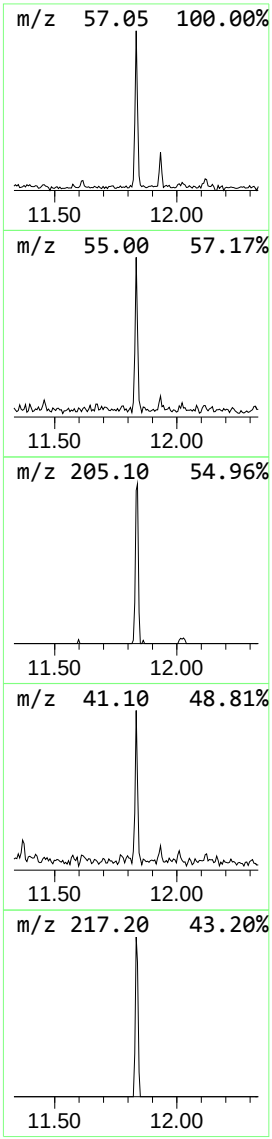
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.833	2.79 ng	130444	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	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	74
3	(1R,3aR,5aR,9aS)-1,4,4,7-Tetrame...	220	C15H24O	104188-25-2	51
4	1-(3-Amino-4,6-dimethylthieno[2,...	220	C11H12N2OS	052505-42-7	38
5	Ethanone, 1-(9-anthracenyl)-	220	C16H12O	000784-04-3	30





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021722\
Data File : BF126930.D
Acq On : 17 Feb 2022 16:49
Operator : CG\JU
Sample : N1573-12
Misc :
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Instrument :
BNA_F
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	4.469	14.8	ng	448428	1	6.928	607158	20.0
Ethanol, 2-(1-m...	5.163	4.7	ng	141918	1	6.928	607158	20.0
2-Propanol, 1-(...	6.722	6.3	ng	191655	1	6.928	607158	20.0
1-Propanol, 2-(...	6.751	6.7	ng	202940	1	6.928	607158	20.0
2-Propanol, 1-(...	6.845	10.9	ng	330376	1	6.928	607158	20.0
1-Hexanol, 2-et...	6.981	20.8	ng	630935	1	6.928	607158	20.0
Benzene, cyclop...	7.104	2.9	ng	87377	1	6.928	607158	20.0
Hexanoic acid, ...	7.575	4.6	ng	190153	2	8.210	833700	20.0
unknown8.110	8.110	2.2	ng	90907	2	8.210	833700	20.0
Nonanoic acid	8.539	3.2	ng	134955	2	8.210	833700	20.0
2,2,4-Trimethyl...	9.157	5.5	ng	239569	3	9.969	877415	20.0
Phenol, 4-(1,1-...	9.380	18.1	ng	792804	3	9.969	877415	20.0
Cyclopentaneace...	10.669	2.8	ng	121169	3	9.969	877415	20.0
7,9-Di-tert-but...	11.833	2.8	ng	130444	4	11.457	934111	20.0