LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082322\
Data File : BG054705.D
Acq On : 23 Aug 2022 13:20
Operator : CG/JU
Sample : N4258-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
280251

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_G\Methods\8270-BG082222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054705.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.223	323	329	339	rVB	120755	193080	2.91%	0.705%
2	5.694	402	409	422	rBV	833595	1395187	21.05%	5.093%
3	7.303	672	683	696	rBV	872537	1516631	22.88%	5.536%
4	8.161	818	829	856	rBV	280184	678269	10.23%	2.476%
5	9.330	1020	1028	1039	rBV	535429	985523	14.87%	3.597%
6	9.548	1057	1065	1076	rBV2	27360	71274	1.08%	0.260%
7	10.981	1303	1309	1316	rVB	281100	518571	7.82%	1.893%
8	13.003	1649	1653	1659	rVB7	56290	90580	1.37%	0.331%
9	13.314	1702	1706	1713	rVB	153789	243428	3.67%	0.889%
10	13.414	1715	1723	1732	rVB	1301469	2164970	32.66%	7.903%
11	13.602	1752	1755	1763	rVB4	120323	189191	2.85%	0.691%
12	14.066	1830	1834	1840	rVB6	180646	306030	4.62%	1.117%
13	14.219	1857	1860	1861	rBV2	96130	107698	1.62%	0.393%
14	14.254	1862	1866	1870	rVV	413756	579446	8.74%	2.115%
15	14.800	1954	1959	1965	rVB2	769375	1461149	22.04%	5.334%
16	16.275	2207	2210	2215	rVB	669612	939983	14.18%	3.431%
17	16.510	2246	2250	2256	rVB	1339615	1913990	28.87%	6.987%
18	17.333	2386	2390	2394	rVB	1423095	2023333	30.52%	7.386%
19	20.071	2851	2856	2863	rBV	4455544	6629040	100.00%	24.198%
20	20.141	2864	2868	2875	rVB	2086313	2845399	42.92%	10.387%
21	21.833	3152	3156	3161	rVB	426690	682584	10.30%	2.492%
22	24.313	3571	3578	3593	rVB	461859	1148146	17.32%	4.191%
23	25.200	3722	3729	3741	rVB2	237118	711492	10.73%	2.597%

Sum of corrected areas: 27394994

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082322\
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Misc :
ALS Vial : 7 Sample Multiplier: 1

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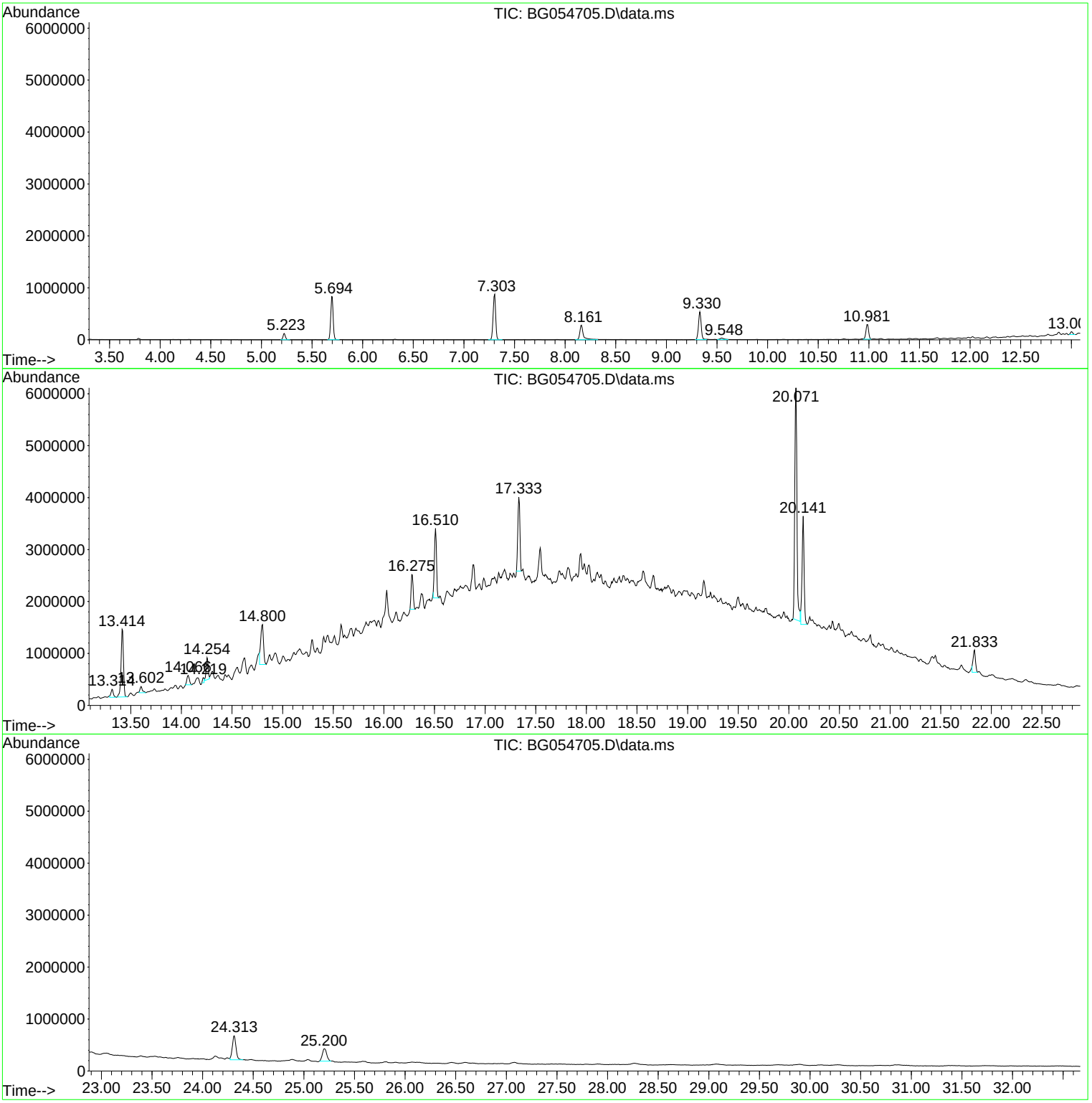
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BG054705.D
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TIC Library : C:\Database\NIST20.L
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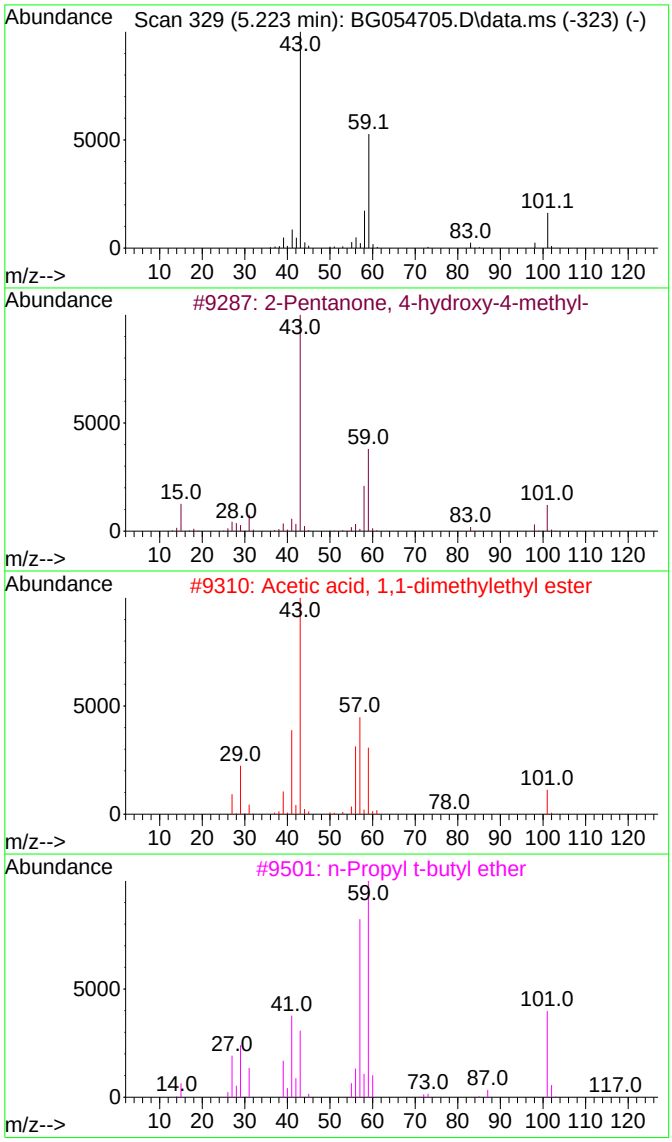
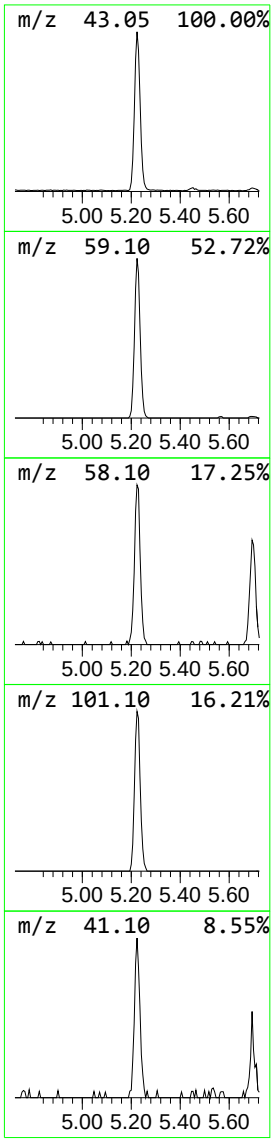
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.223	5.69 ng	193080	1,4-Dichlorobenzene-d4	8.161

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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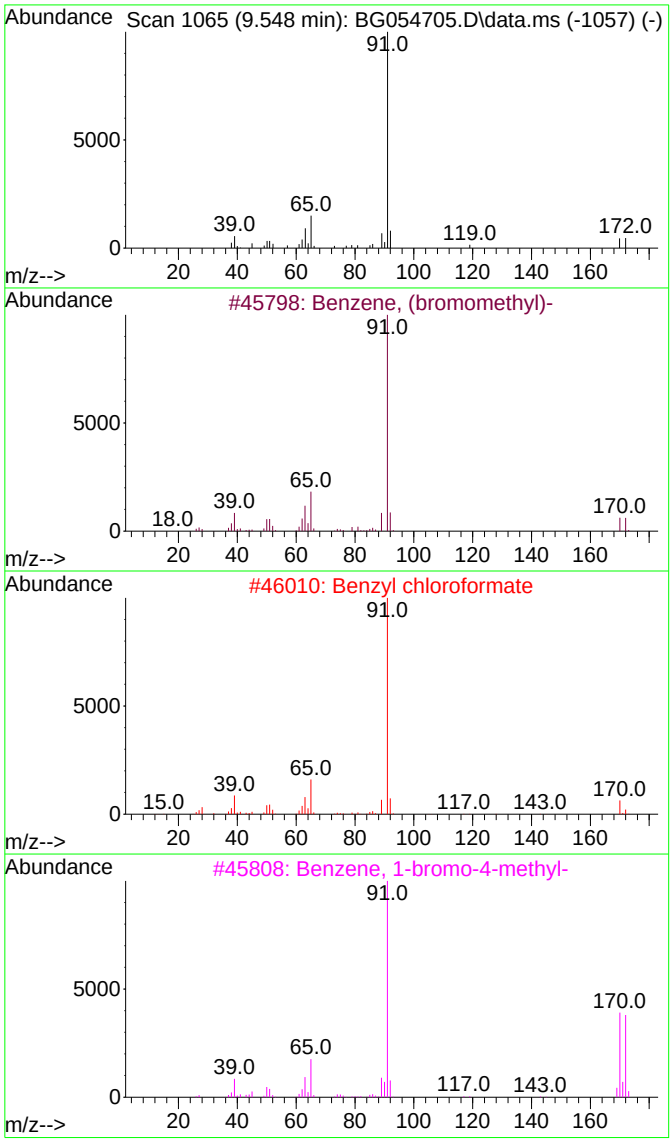
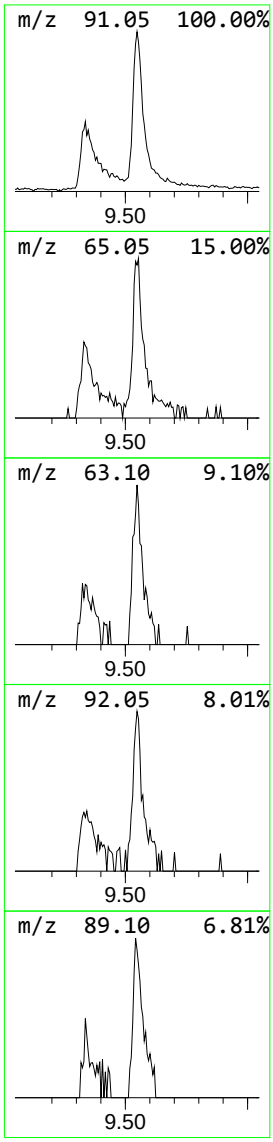
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Benzene, (bromomethyl)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.548	2.10 ng	71274	1,4-Dichlorobenzene-d4	8.161

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (bromomethyl)-	170	C7H7Br	000100-39-0	93
2	Benzyl chloroformate	170	C8H7ClO2	000501-53-1	90
3	Benzene, 1-bromo-4-methyl-	170	C7H7Br	000106-38-7	78
4	Triethylbenzylammonium bromide	271	C13H22BrN	005197-95-5	78
5	Benzene, [(methylsulfonyl)methyl]-	170	C8H10O2S	003112-90-1	72





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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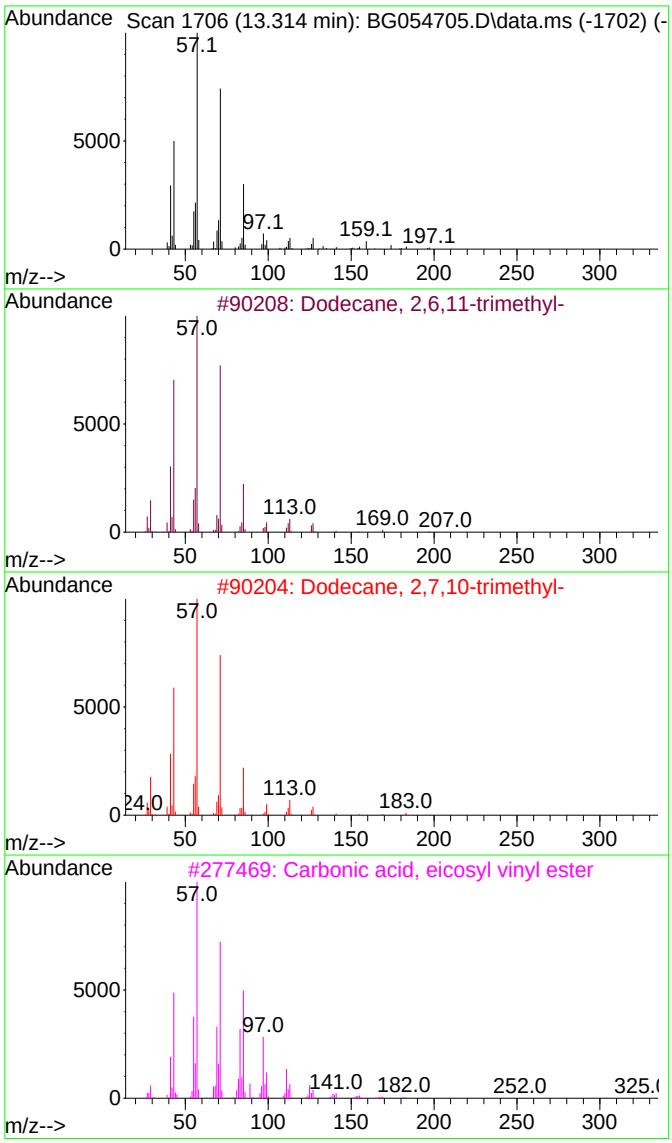
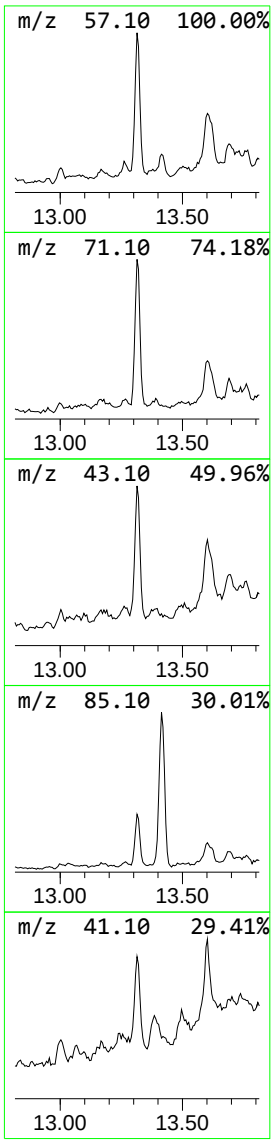
****

Peak Number 3 Dodecane, 2,6,11-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.314	3.33 ng	243428	Acenaphthene-d10	14.795

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	86
2	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	80
3	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	72
4	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	64
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	64





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Misc :
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Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082222.M
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TIC Library : C:\Database\NIST20.L
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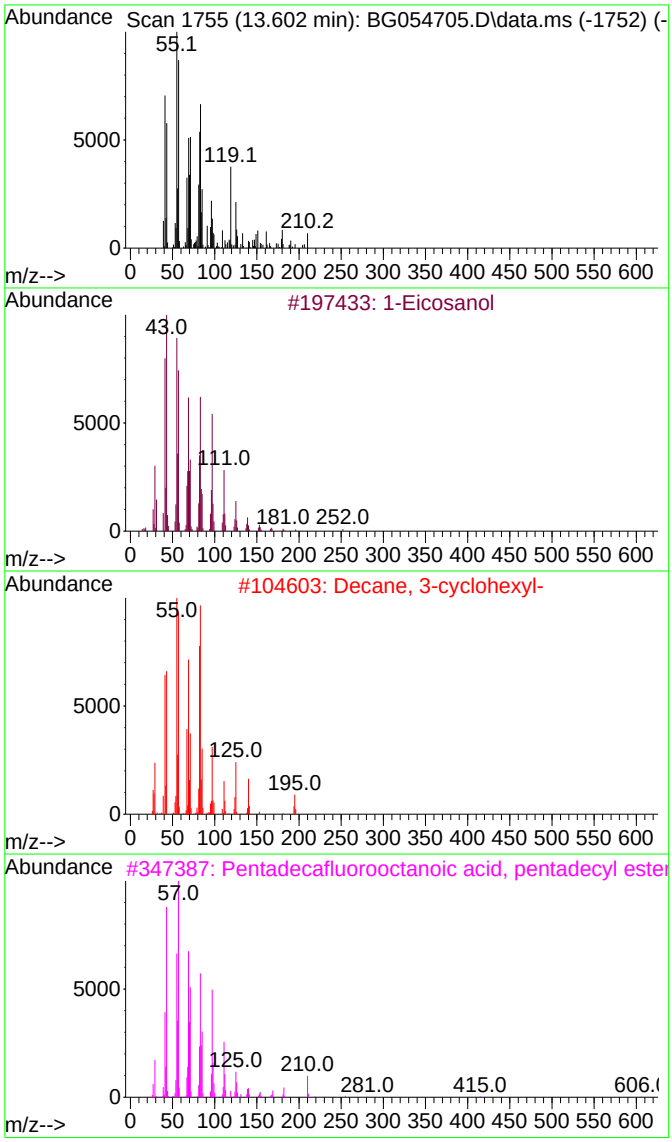
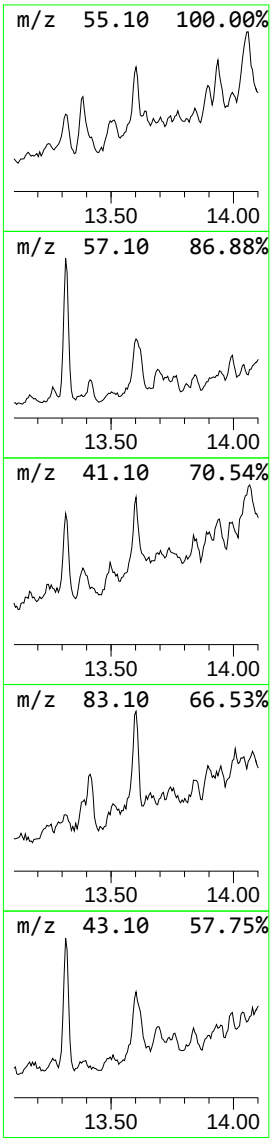
****

Peak Number 4 1-Eicosanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.602	2.59 ng	189191	Acenaphthene-d10	14.795

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Eicosanol	298	C20H42O	000629-96-9	72
2	Decane, 3-cyclohexyl-	224	C16H32	013151-74-1	49
3	Pentadecafluorooctanoic acid, pe...	624	C23H31F15O2	1000406-04-5	43
4	Cyclohexane, 1,1'-methylenebis-	180	C13H24	003178-23-2	35
5	Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	25





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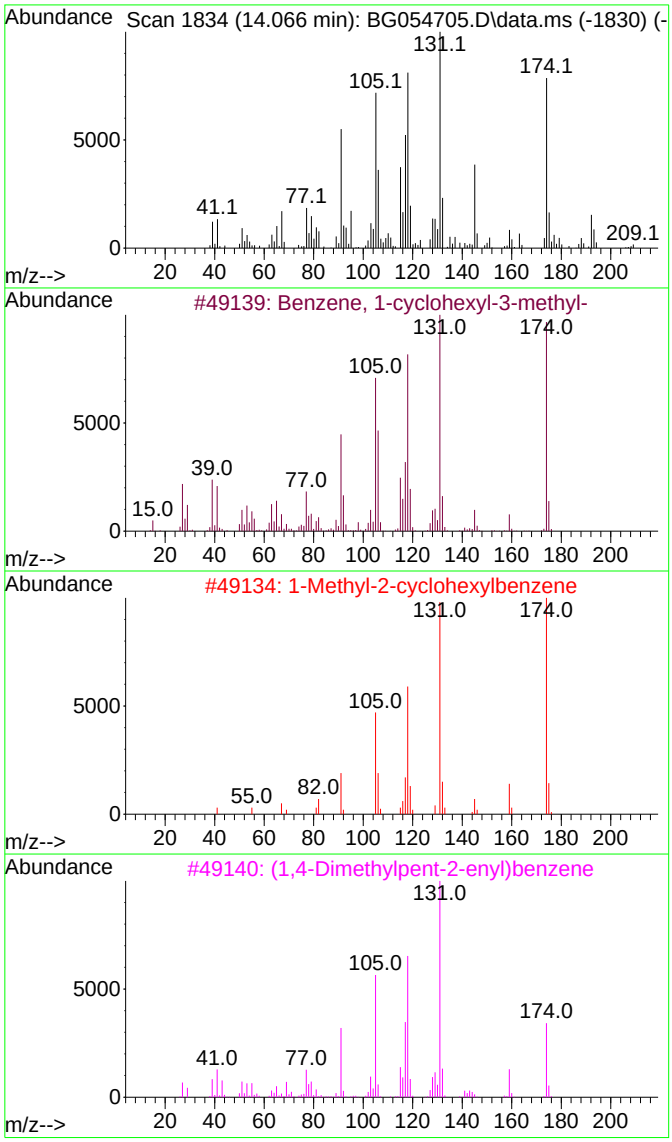
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

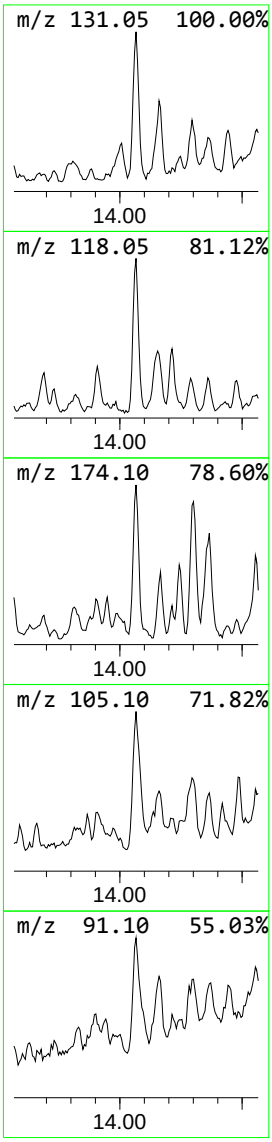
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 1-cyclohexyl-3-met... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.066	4.19 ng	306030	Acenaphthene-d10	14.795

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-cyclohexyl-3-methyl-	174	C13H18	004575-46-6	81
2	1-Methyl-2-cyclohexylbenzene	174	C13H18	004501-35-3	74
3	(1,4-Dimethylpent-2-enyl)benzene	174	C13H18	1000184-97-9	62
4	4-Phenylcyclohexanone	174	C12H14O	004894-75-1	43
5	2-Naphthalenol, 3-methoxy-	174	C11H10O2	018515-11-2	30





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Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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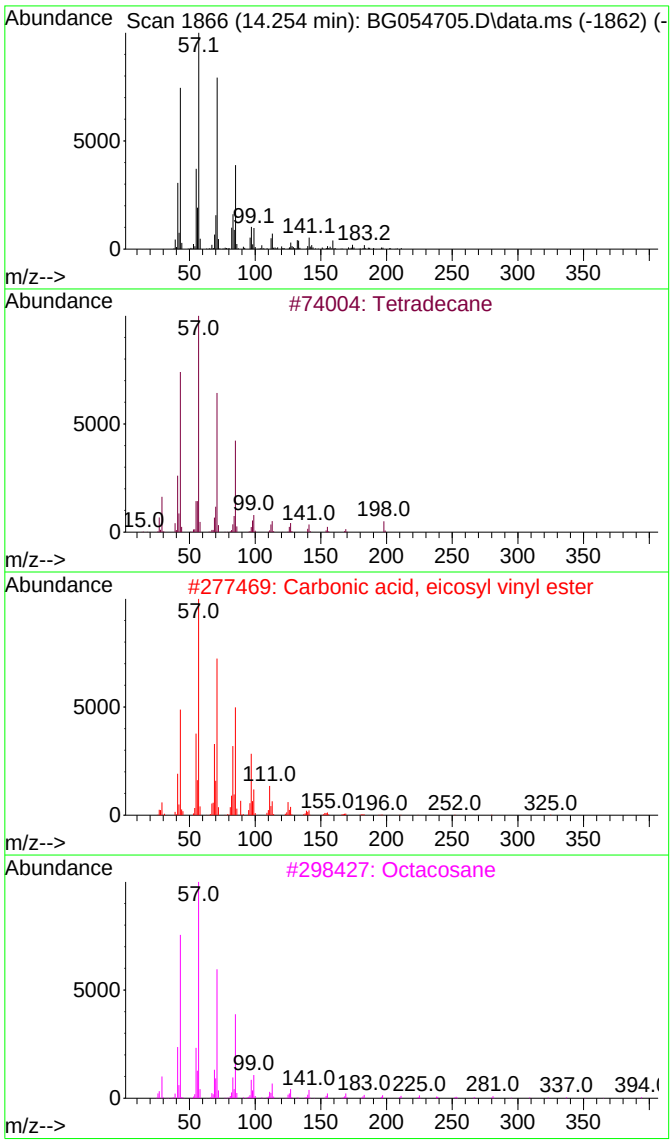
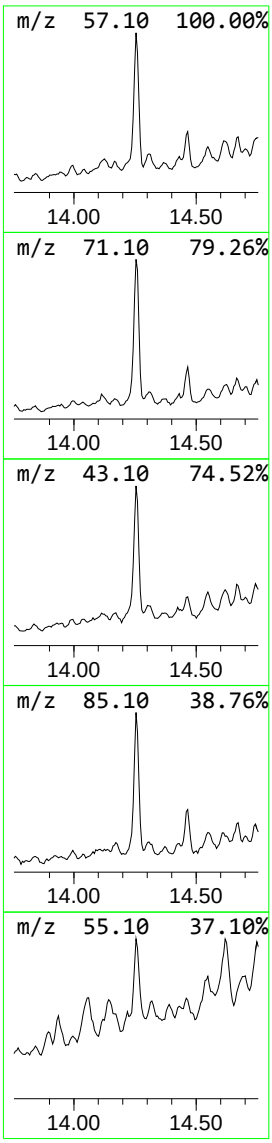
****

Peak Number 6 Tetradecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.254	7.93 ng	579446	Acenaphthene-d10	14.795

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	80
2	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	72
3	Octacosane	394	C28H58	000630-02-4	72
4	Decane, 5-propyl-	184	C13H28	017312-62-8	68
5	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	64





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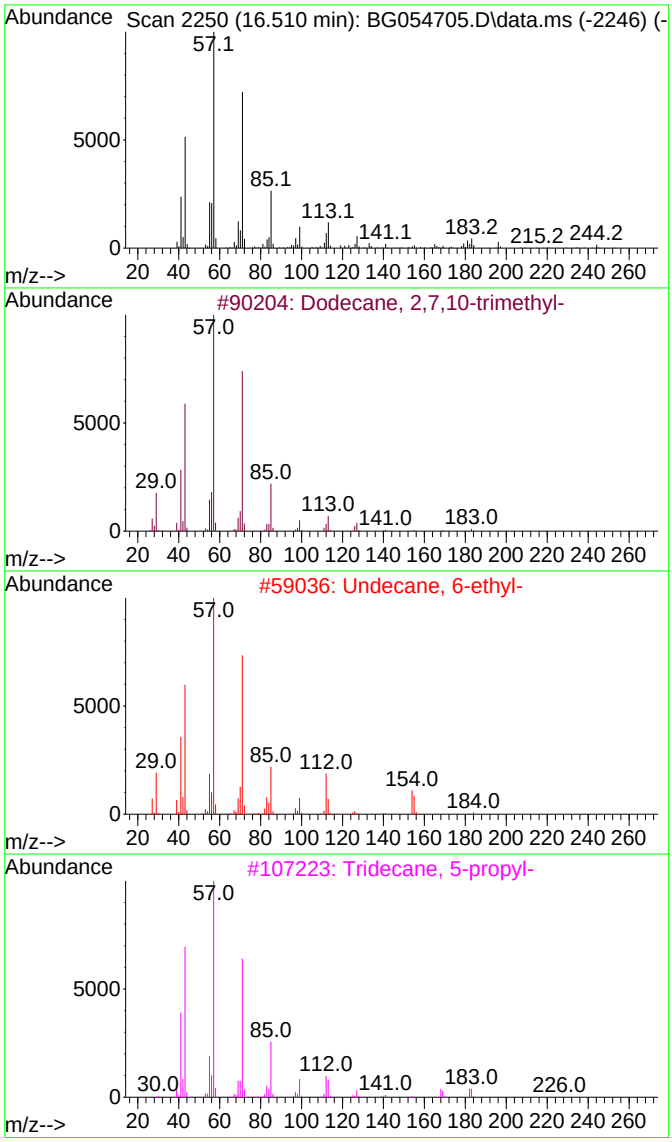
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

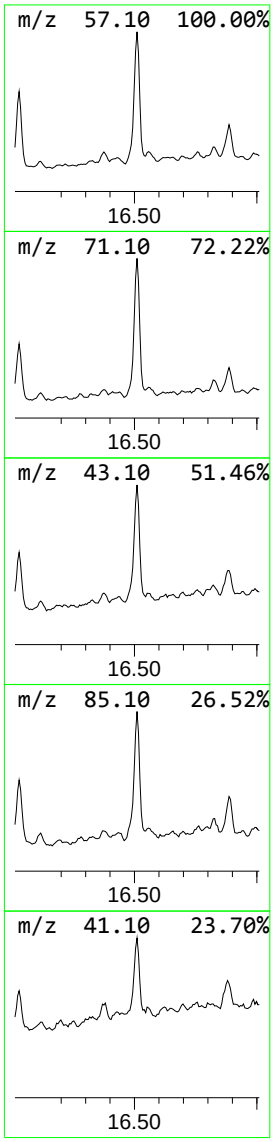
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Dodecane, 2,7,10-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.510	18.92 ng	1913990	Phenanthrene-d10	17.544

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	86
2	Undecane, 6-ethyl-	184	C13H28	017312-60-6	83
3	Tridecane, 5-propyl-	226	C16H34	055045-11-9	80
4	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	80
5	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	80





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TIC Library : C:\Database\NIST20.L
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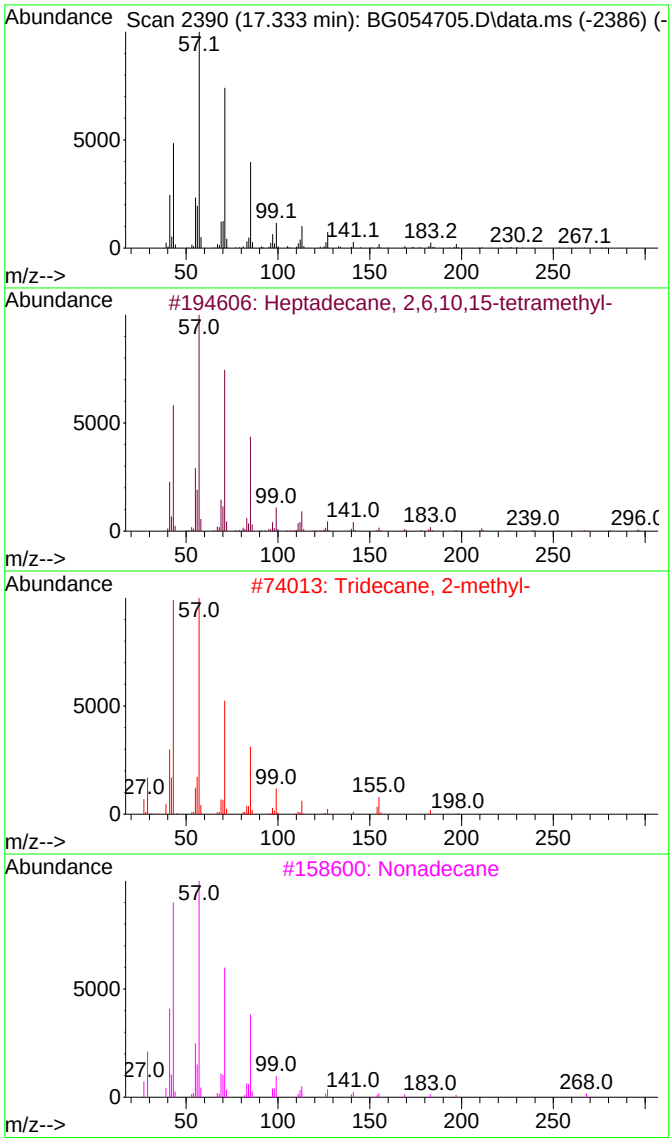
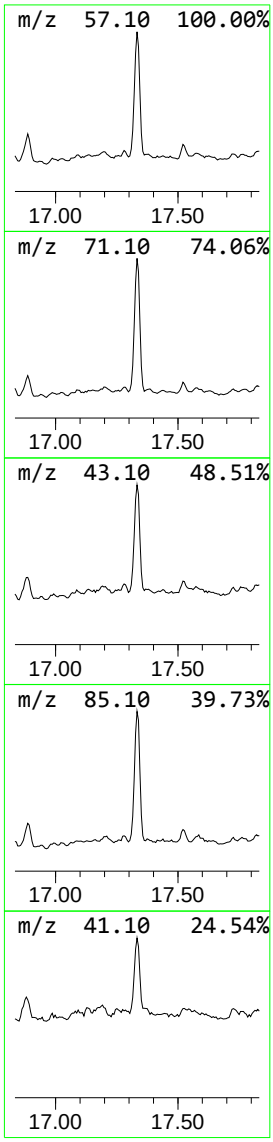
****
Peak Number 8 Heptadecane, 2,6,10,15-tetr... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.333	20.00 ng	2023330	Phenanthrene-d10	17.544

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91
2	Tridecane, 2-methyl-	198	C14H30	001560-96-9	90
3	Nonadecane	268	C19H40	000629-92-5	90
4	Eicosane	282	C20H42	000112-95-8	86
5	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	80





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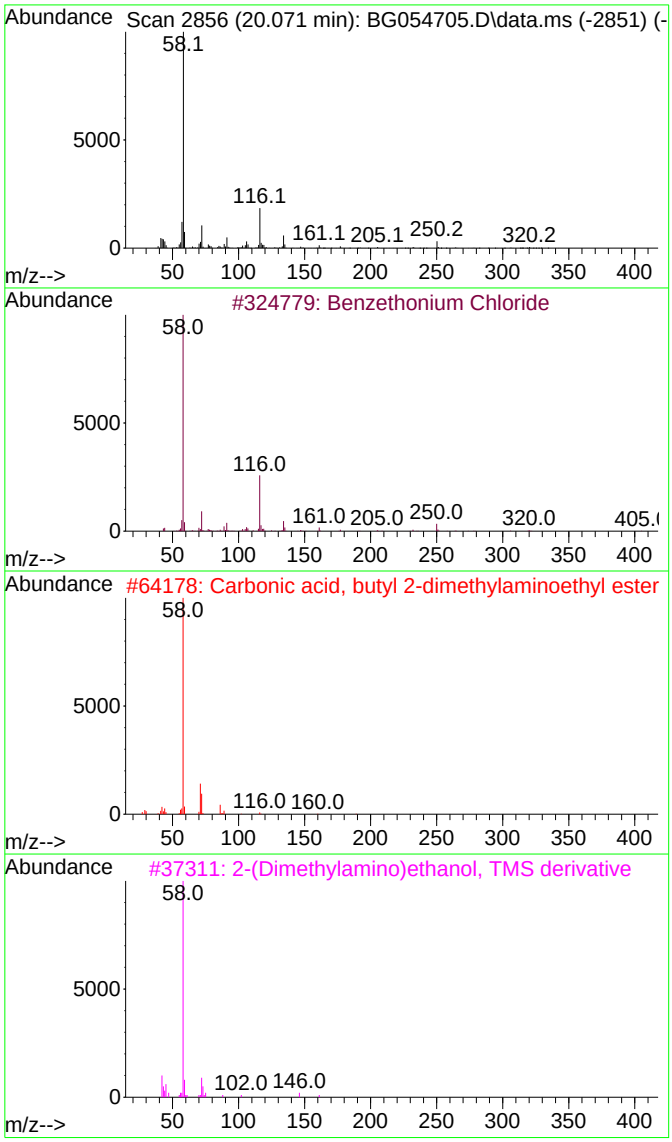
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

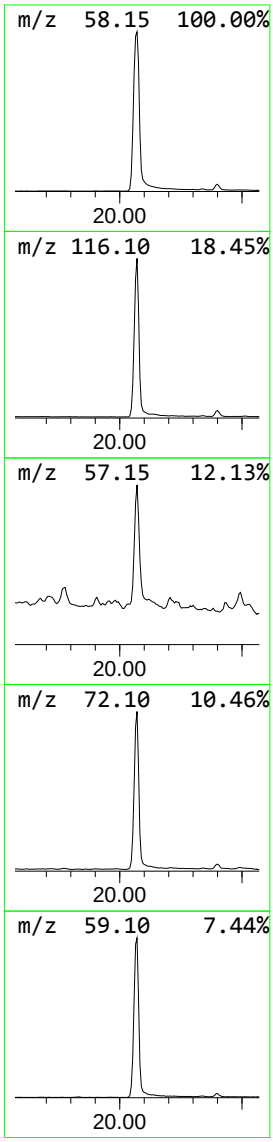
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzethonium Chloride Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.071	194.23 ng	6629040	Chrysene-d12	21.833

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzethonium Chloride	447	C27H42ClNO2	000121-54-0	87
2	Carbonic acid, butyl 2-dimethyla...	189	C9H19NO3	1000331-41-4	59
3	2-(Dimethylamino)ethanol, TMS de...	161	C7H19NOSi	016654-64-1	59
4	Acetone, 1-[4-(dimethylaminoetho...	221	C13H19NO2	086608-11-9	53
5	N,N-Dimethyl-2-methoxyethylamine	103	C5H13NO	003030-44-2	53





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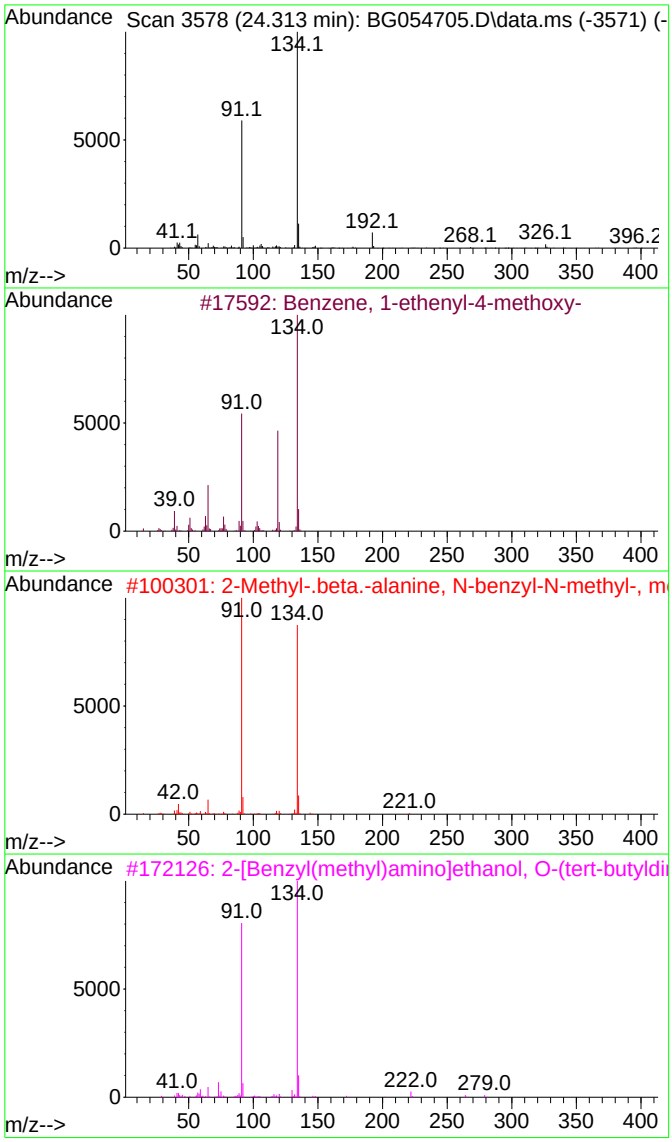
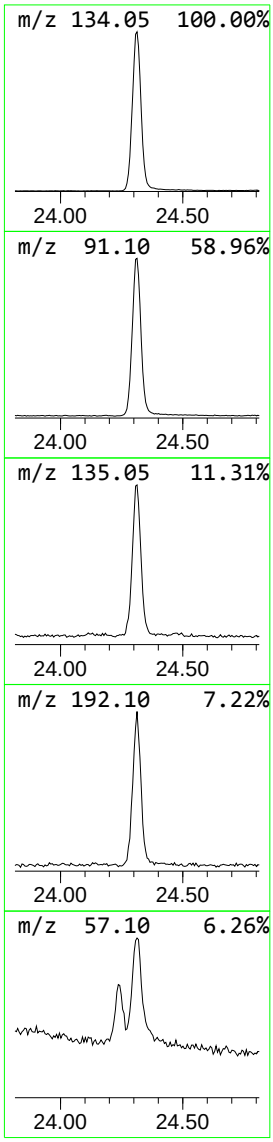
****
Peak Number 10 Benzene, 1-ethenyl-4-methoxy- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.313	32.27 ng	1148150	Perylene-d12	25.206

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-4-methoxy-	134	C9H10O	000637-69-4	72
2	2-Methyl-.beta.-alanine, N-benzy...	221	C13H19NO2	1000452-75-6	56
3	2-[Benzyl(methyl)amino]ethanol, ...	279	C16H29NOSi	1000481-09-4	56
4	Dodecylmethylbenzylamine	289	C20H35N	068397-57-9	56
5	7-Methoxy-3-(p-methoxyphenyl)-4-...	284	C17H16O4	015236-11-0	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082322\
Data File : BG054705.D
Acq On : 23 Aug 2022 13:20
Operator : CG/JU
Sample : N4258-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
280251

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082222.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
2-Pentanone, 4-...	5.223	5.7	ng	193080	1	8.161	678269	20.0
Benzene, (bromo...	9.548	2.1	ng	71274	1	8.161	678269	20.0
Dodecane, 2,6,1...	13.314	3.3	ng	243428	3	14.795	1461150	20.0
1-Eicosanol	13.602	2.6	ng	189191	3	14.795	1461150	20.0
Benzene, 1-cycl...	14.066	4.2	ng	306030	3	14.795	1461150	20.0
Tetradecane	14.254	7.9	ng	579446	3	14.795	1461150	20.0
Dodecane, 2,7,1...	16.510	18.9	ng	1913990	4	17.544	2023330	20.0
Heptadecane, 2,...	17.333	20.0	ng	2023330	4	17.544	2023330	20.0
Benzethonium Ch...	20.071	194.2	ng	6629040	5	21.833	682584	20.0
Benzene, 1-ethe...	24.313	32.3	ng	1148150	6	25.206	711492	20.0