LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081122\
Data File : BG054602.D
Acq On : 11 Aug 2022 13:04
Operator : CG/JU
Sample : N3971-15
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
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_G\Methods\8270-BG071522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054602.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.087	11	17	32	rVB	251211	410974	22.32%	6.584%
2	4.403	236	241	254	rVB	52543	91028	4.94%	1.458%
3	5.049	345	351	361	rBV2	15002	27777	1.51%	0.445%
4	5.560	432	438	451	rVB	110113	198988	10.81%	3.188%
5	6.600	610	615	624	rVB2	14097	24469	1.33%	0.392%
6	7.176	707	713	723	rBV2	70469	134275	7.29%	2.151%
7	7.969	841	848	854	rBV2	44835	77656	4.22%	1.244%
8	9.139	1040	1047	1056	rBV	148473	274192	14.89%	4.392%
9	10.778	1319	1326	1340	rBB	56134	107840	5.86%	1.728%
10	11.724	1481	1487	1497	rVB3	9773	23831	1.29%	0.382%
11	13.228	1736	1743	1753	rBV	468939	758534	41.20%	12.151%
12	13.463	1777	1783	1795	rVB	147924	232526	12.63%	3.725%
13	14.614	1972	1979	1985	rBV	115714	185571	10.08%	2.973%
14	16.107	2227	2233	2248	rBV	479664	775147	42.10%	12.417%
15	17.358	2439	2446	2455	rBV	175230	277696	15.08%	4.449%
16	18.016	2552	2558	2562	rVB	22505	28127	1.53%	0.451%
17	19.967	2884	2890	2897	rBV	1362287	1841321	100.00%	29.497%
18	21.624	3166	3172	3181	rVB	224699	372632	20.24%	5.969%
19	23.052	3412	3415	3423	rVB9	11550	19657	1.07%	0.315%
20	24.832	3708	3718	3731	rVB	130223	380141	20.65%	6.090%

Sum of corrected areas: 6242382

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BNA_G
ClientSampleId :
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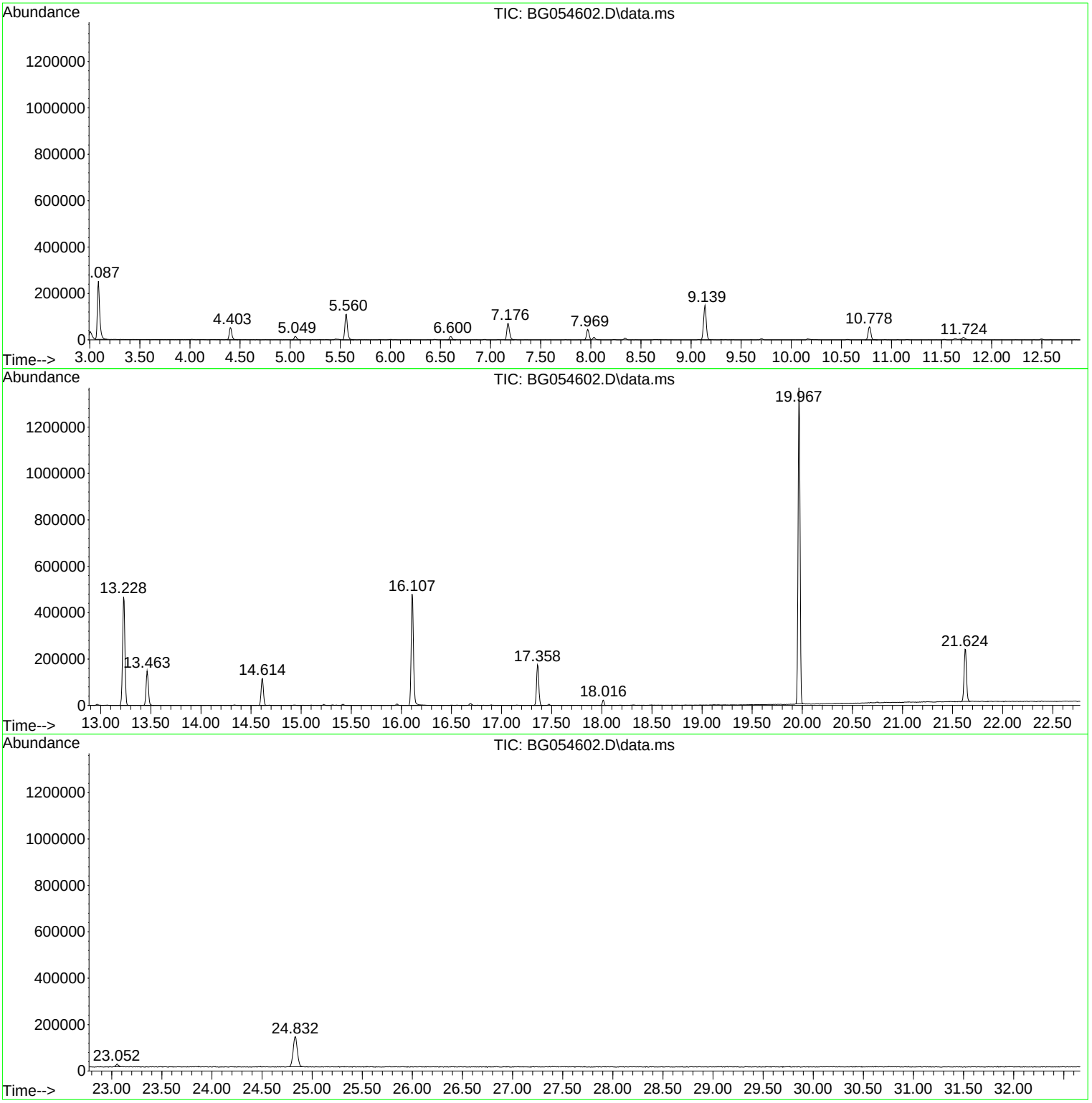
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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TIC Library : C:\Database\NIST20.L
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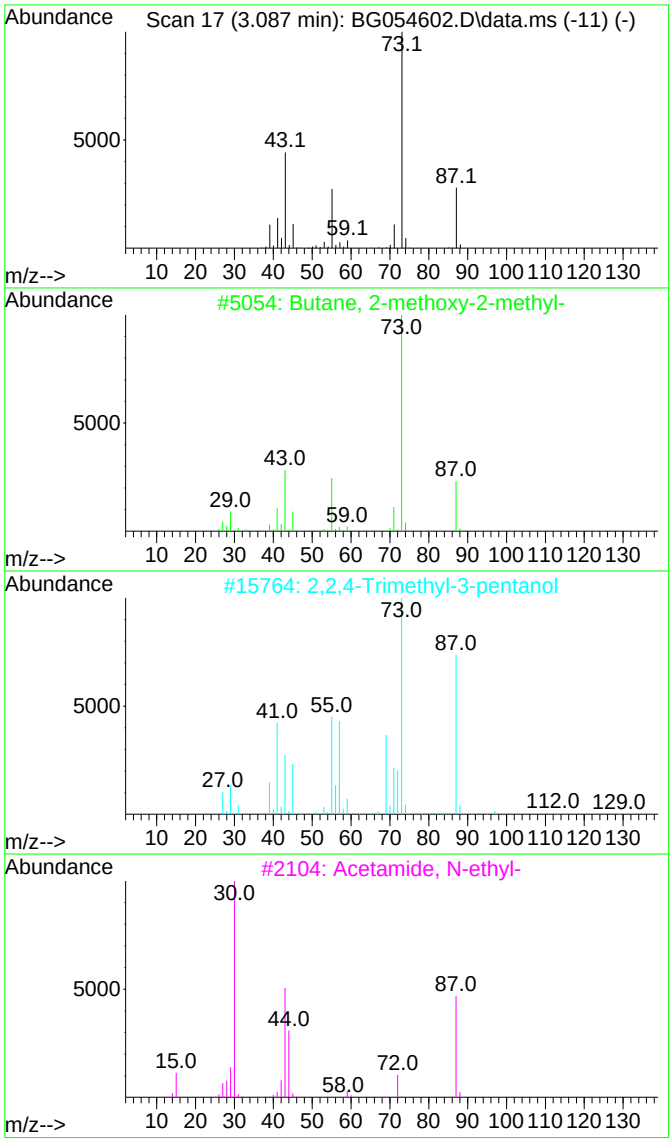
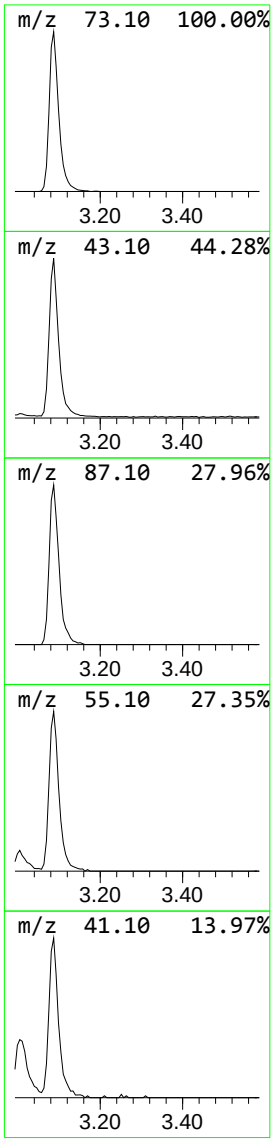
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.087	105.85 ng	410974	1,4-Dichlorobenzene-d4	7.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	35
4	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	16





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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
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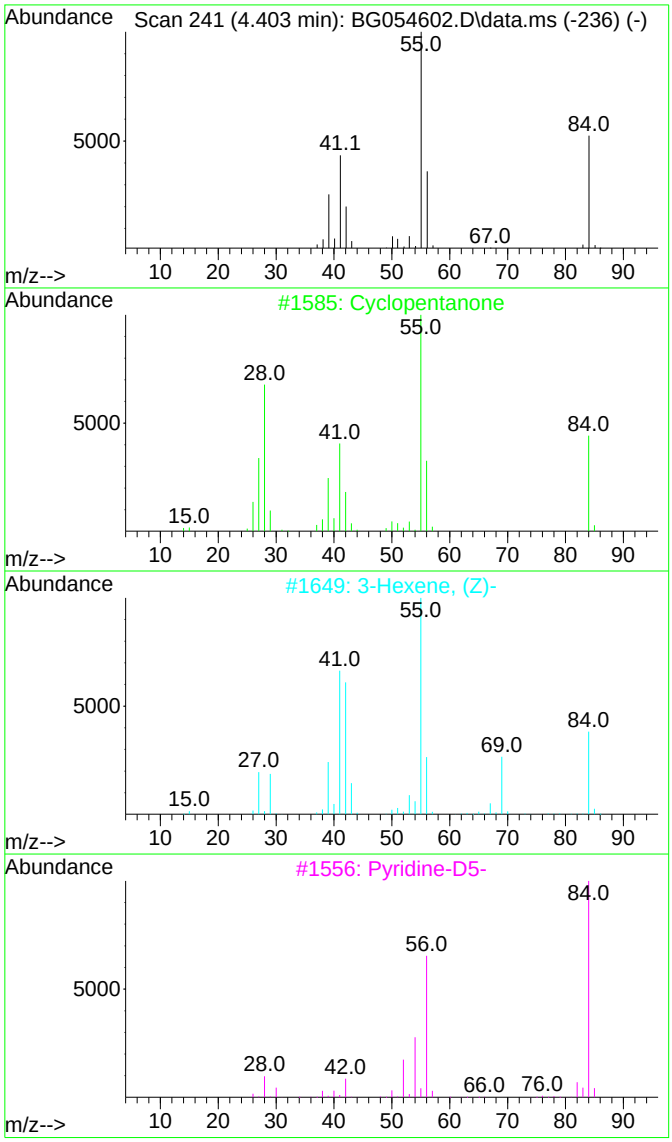
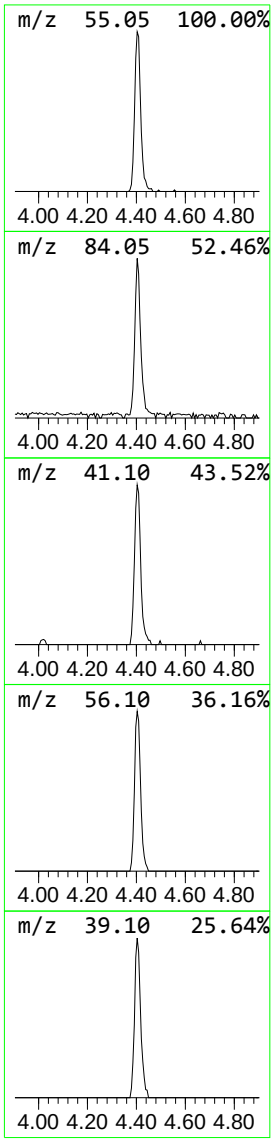
Peak Number 2 Cyclopentanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.403	23.44 ng	91028	1,4-Dichlorobenzene-d4	7.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanone	84	C5H8O	000120-92-3	91
2	3-Hexene, (Z)-	84	C6H12	007642-09-3	50
3	Pyridine-D5-	84	C5D5N	007291-22-7	49
4	2(5H)-Furanone	84	C4H4O2	000497-23-4	49
5	2-Hexene, (Z)-	84	C6H12	007688-21-3	42





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ClientSampleId :
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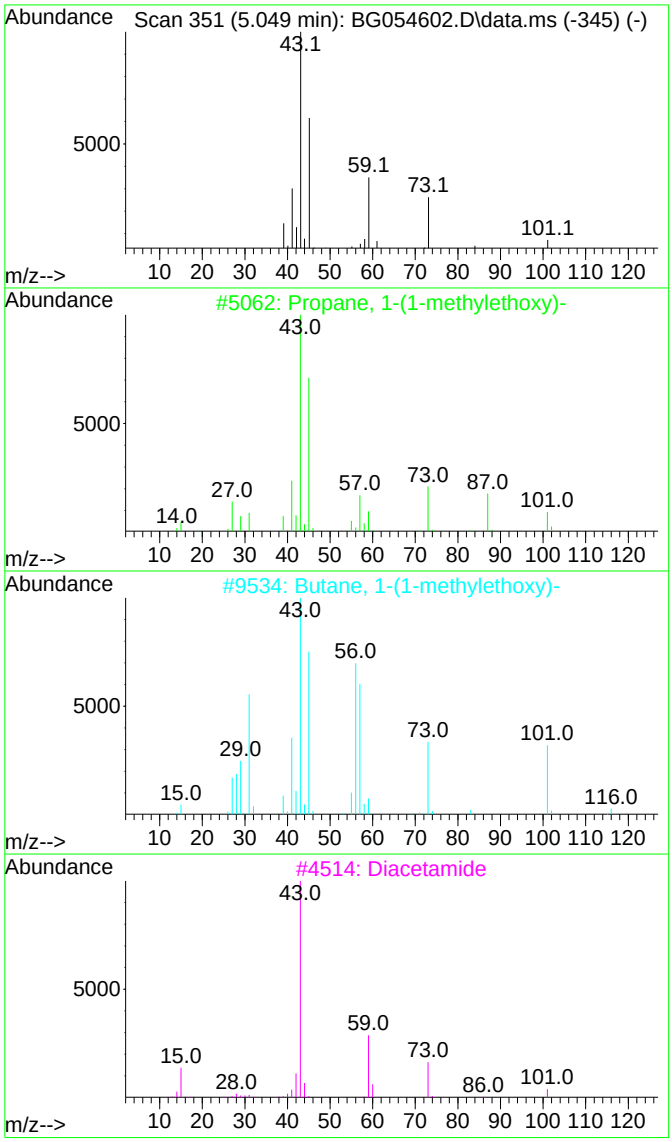
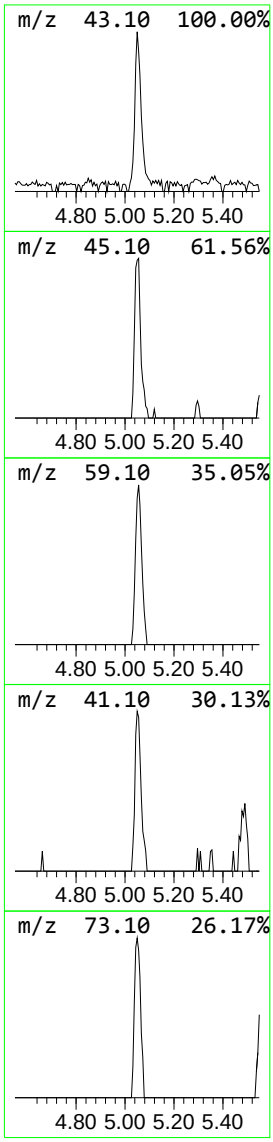
Peak Number 3 unknown5.049 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.049	7.15 ng	27777	1,4-Dichlorobenzene-d4	7.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	42
2	Butane, 1-(1-methylethoxy)-	116	C7H16O	001860-27-1	42
3	Diacetamide	101	C4H7NO2	000625-77-4	38
4	2-Methyoxirane-2-carboxylic acid...	116	C5H8O3	1010306-64-8	28
5	Oxirane, trimethyl-	86	C5H10O	005076-19-7	25





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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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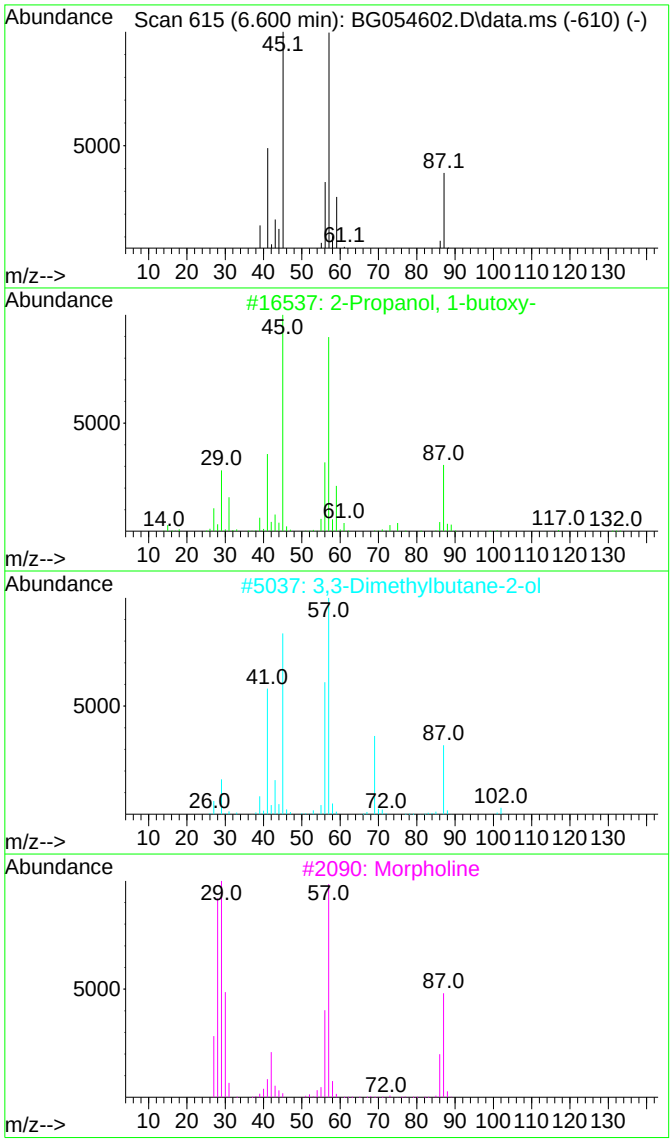
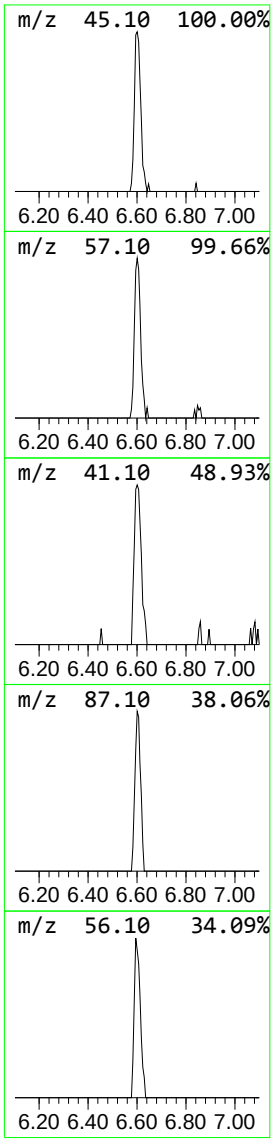
Peak Number 4 2-Propanol, 1-butoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.600	6.30 ng	24469	1,4-Dichlorobenzene-d4	7.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	78
2	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	38
3	Morpholine	87	C4H9NO	000110-91-8	25
4	1-Pentanamine	87	C5H13N	000110-58-7	9
5	Ethanol, 2-(vinyloxy)-	88	C4H8O2	000764-48-7	9





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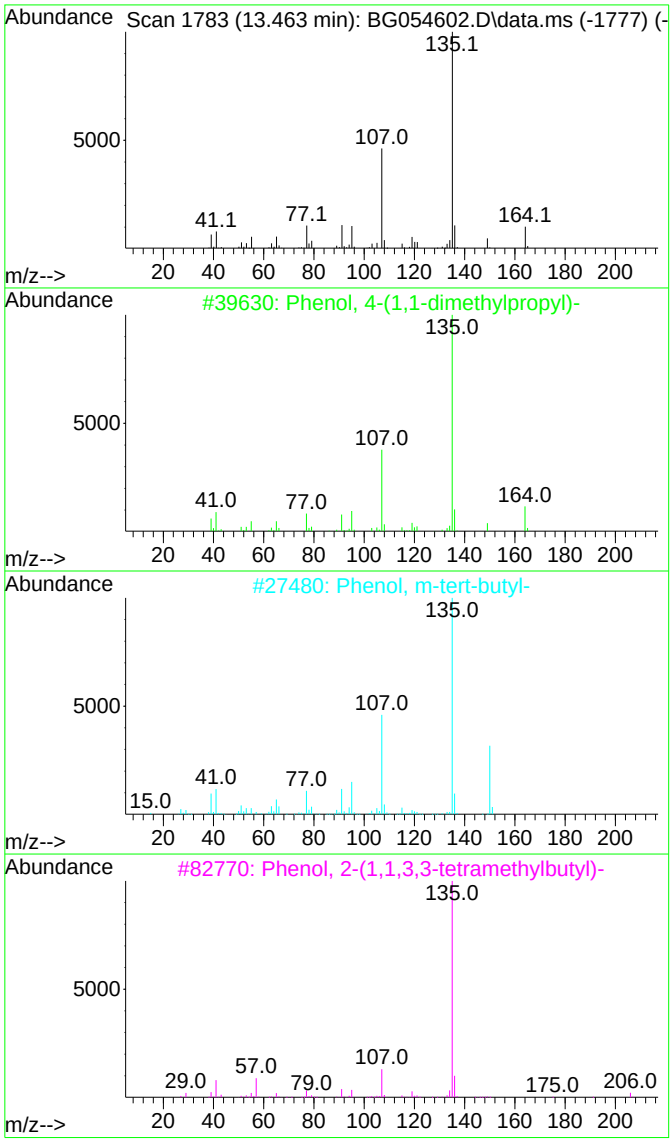
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

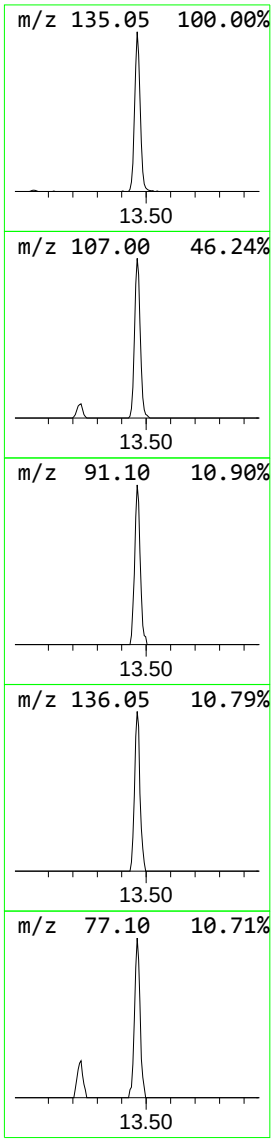
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Phenol, 4-(1,1-dimethylprop... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.463	25.06 ng	232526	Acenaphthene-d10	14.615

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	95
2	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	72
3	Phenol, 2-(1,1,3,3-tetramethylbu...	206	C14H22O	003884-95-5	64
4	4,4'-(1,2-diethylethylene)diphenol	270	C18H22O2	005635-50-7	64
5	Hexestrol	270	C18H22O2	000084-16-2	64





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TIC Library : C:\Database\NIST20.L
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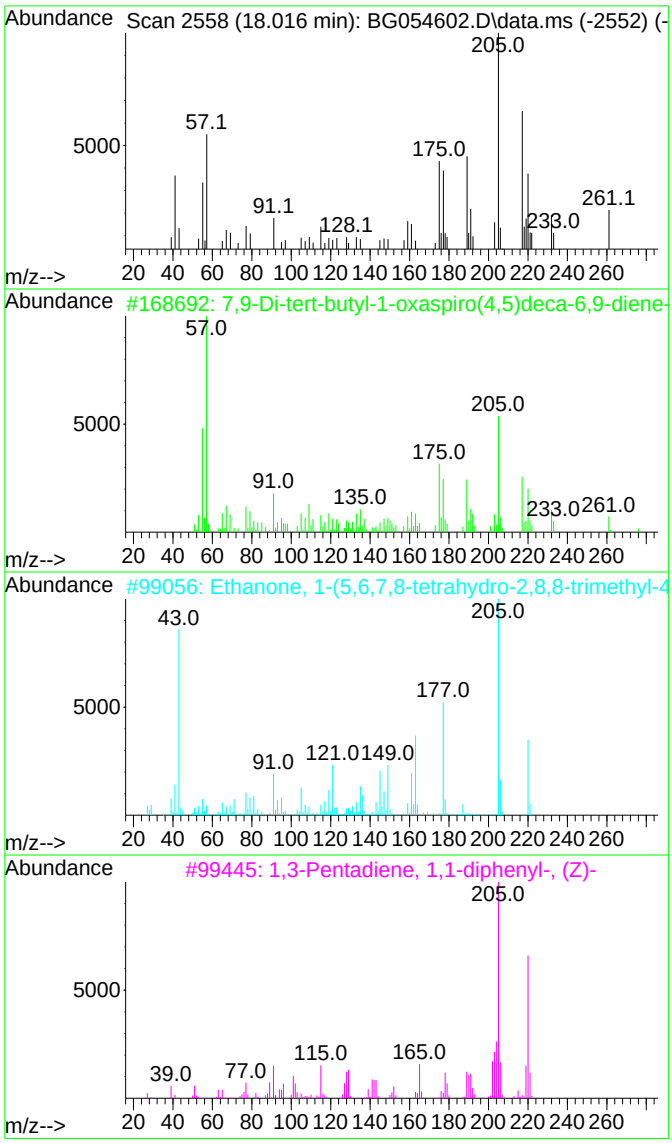
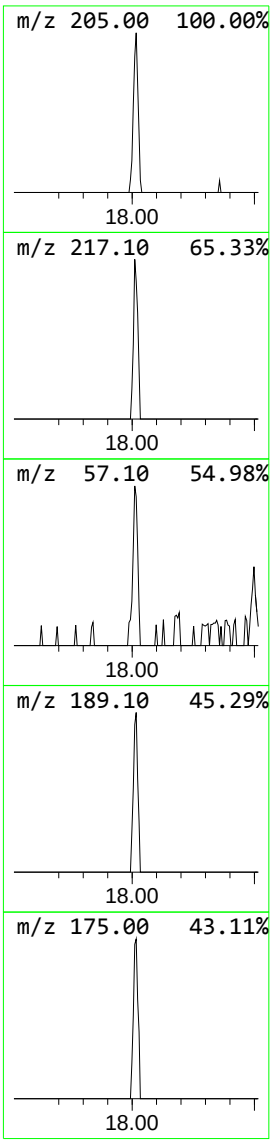
Peak Number 6 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.016	2.03 ng	28127	Phenanthrene-d10	17.358

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	72
2	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	38
3	1,3-Pentadiene, 1,1-diphenyl-, (Z)-	220	C17H16	015295-31-5	38
4	1-(3-Amino-4,6-dimethylthieno[2,...	220	C11H12N2OS	052505-42-7	35
5	2,3-Quinoxalinedione, 6-amino-1,...	205	C10H11N3O2	1010338-06-6	30





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...	3.087	105.8	ng	410974	1	7.969	77656	20.0
Cyclopentanone	4.403	23.4	ng	91028	1	7.969	77656	20.0
unknown5.049	5.049	7.2	ng	27777	1	7.969	77656	20.0
2-Propanol, 1-b...	6.600	6.3	ng	24469	1	7.969	77656	20.0
Phenol, 4-(1,1-...	13.463	25.1	ng	232526	3	14.615	185571	20.0
7,9-Di-tert-but...	18.016	2.0	ng	28127	4	17.358	277696	20.0