LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021722\
Data File : BP009201.D
Acq On : 17 Feb 2022 18:25
Operator : CG/JU
Sample : N1575-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-15

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_P\Methods\8270E-BP020722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP009201.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.263	212	217	238	rVB	300198	485501	2.33%	0.609%
2	4.904	321	326	334	rBV2	121747	218886	1.05%	0.274%
3	5.375	400	406	440	rVB	2039070	3708559	17.79%	4.650%
4	6.975	671	678	701	rBV	1144091	2556055	12.26%	3.205%
5	7.328	733	738	743	rBV	157338	260532	1.25%	0.327%
6	7.381	743	747	757	rVB	158918	287437	1.38%	0.360%
7	7.575	774	780	805	rVB	224730	486692	2.34%	0.610%
8	7.775	807	814	822	rVV	799322	1400060	6.72%	1.756%
9	7.845	822	826	845	rVB	117316	236566	1.14%	0.297%
10	8.939	1000	1012	1038	rBV	2603508	4997374	23.98%	6.266%
11	10.569	1282	1289	1310	rBV	958280	1973363	9.47%	2.474%
12	12.775	1657	1664	1679	rBV	226367	429664	2.06%	0.539%
13	13.039	1701	1709	1730	rBV	8637358	14005096	67.20%	17.561%
14	13.269	1740	1748	1768	rVB	1119029	1917644	9.20%	2.405%
15	14.422	1936	1944	1955	rBV	1777190	2934709	14.08%	3.680%
16	15.245	2076	2084	2095	rVB2	227333	399826	1.92%	0.501%
17	15.792	2172	2177	2189	rBV	164377	271452	1.30%	0.340%
18	15.921	2192	2199	2217	rBV	6914651	11051285	53.02%	13.857%
19	17.180	2407	2413	2430	rBV	2267432	3618168	17.36%	4.537%
20	17.845	2521	2526	2532	rBV2	268018	353965	1.70%	0.444%
21	19.745	2843	2849	2862	rBV	14981338	20841678	100.00%	26.133%
22	21.062	3070	3073	3080	rBV	124699	213822	1.03%	0.268%
23	21.280	3105	3110	3121	rBV	2493284	3754330	18.01%	4.708%
24	23.668	3510	3516	3534	rVB2	1419509	3349006	16.07%	4.199%

Sum of corrected areas: 79751670

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021722\
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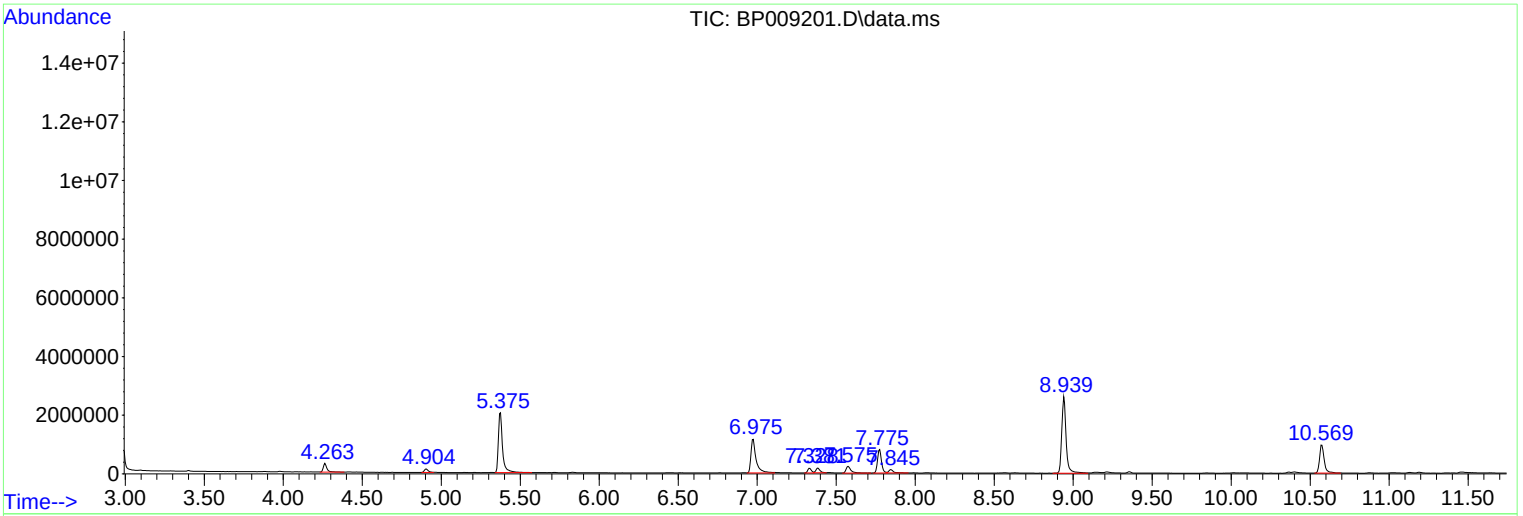
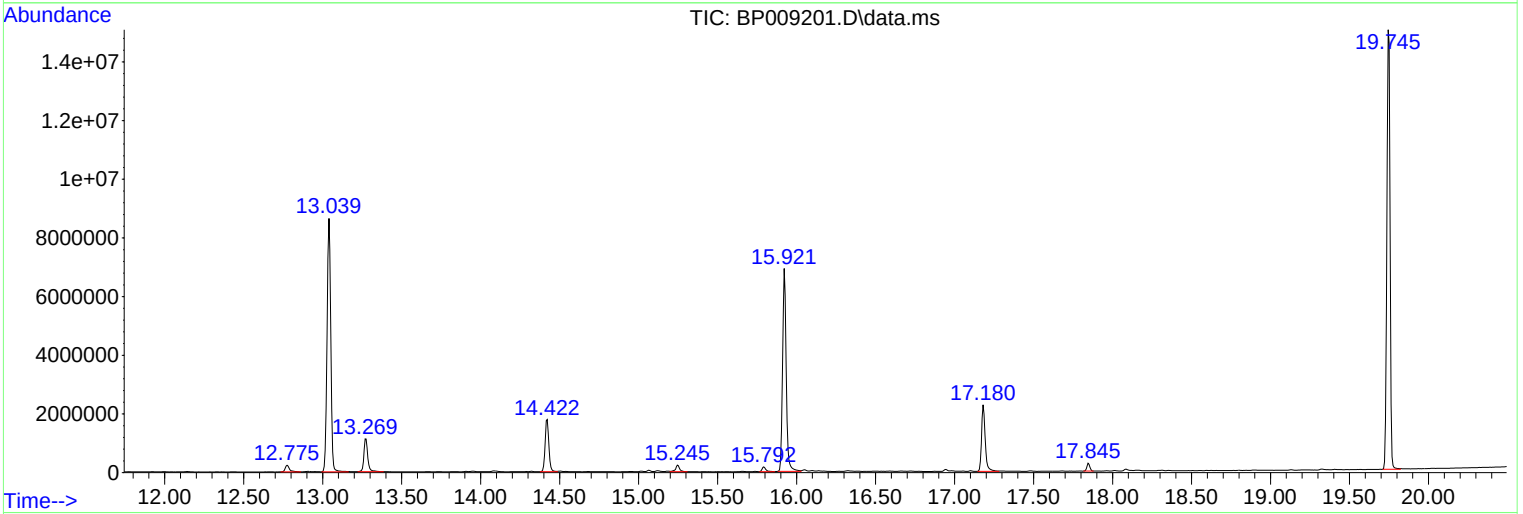
Misc :
ALS Vial : 11 Sample Multiplier: 1

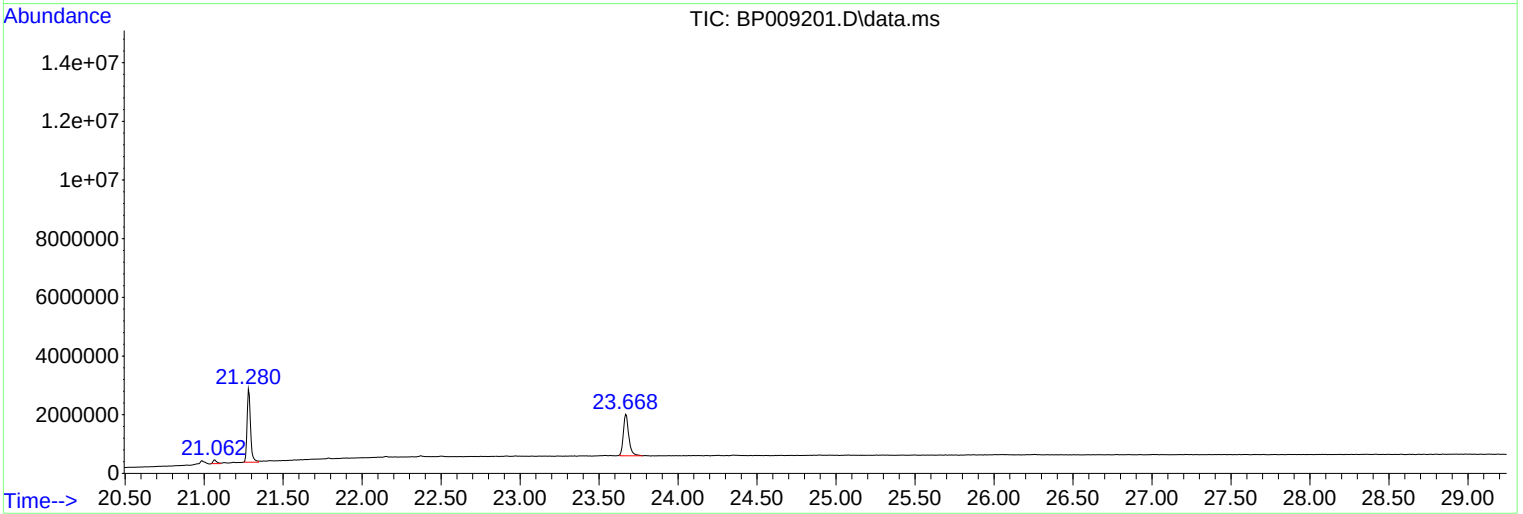
Instrument :
BNA_P
ClientSampleId :
MW-15

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.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 : BP009201.D
Acq On : 17 Feb 2022 18:25
Operator : CG/JU
Sample : N1575-07
Misc :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

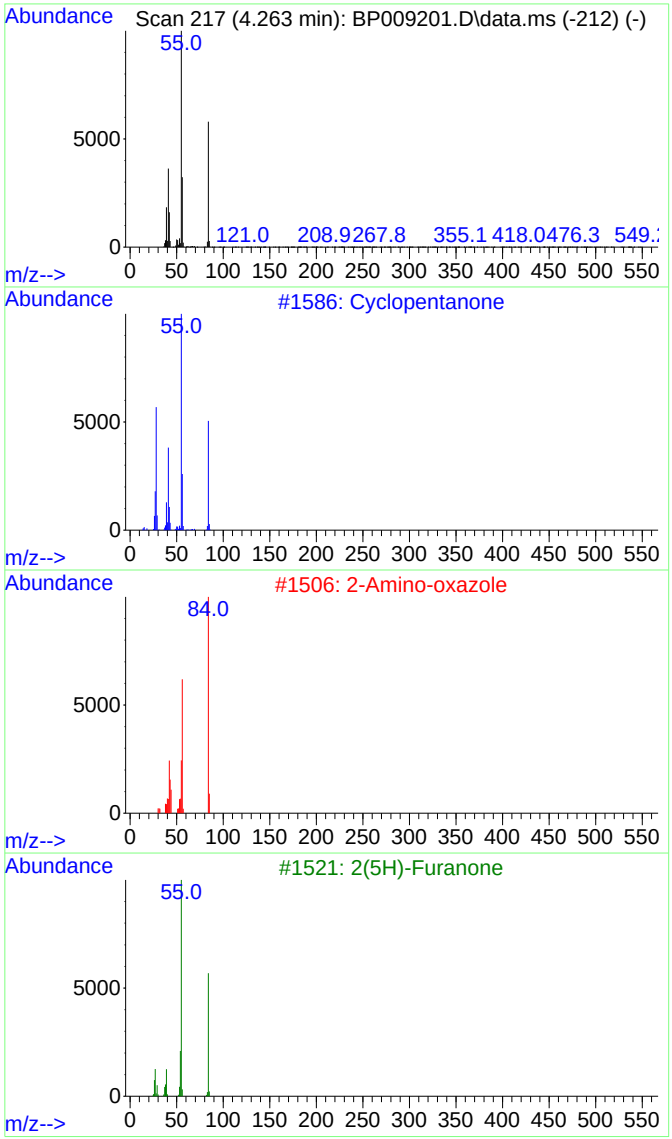
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

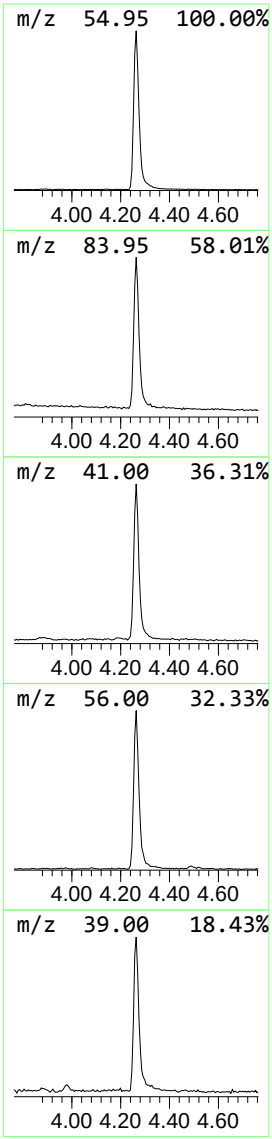
****

Peak Number 1 Cyclopentanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.263	6.94 ng	485501	1,4-Dichlorobenzene-d4	7.775

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanone	84	C5H8O	000120-92-3	91
2	2-Amino-oxazole	84	C3H4N2O	004570-45-0	53
3	2(5H)-Furanone	84	C4H4O2	000497-23-4	52
4	3-Aminoisoxazole	84	C3H4N2O	001750-42-1	45
5	2H-Pyran, 3,4-dihydro-	84	C5H8O	000110-87-2	45





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Data File : BP009201.D
Acq On : 17 Feb 2022 18:25
Operator : CG/JU
Sample : N1575-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-15

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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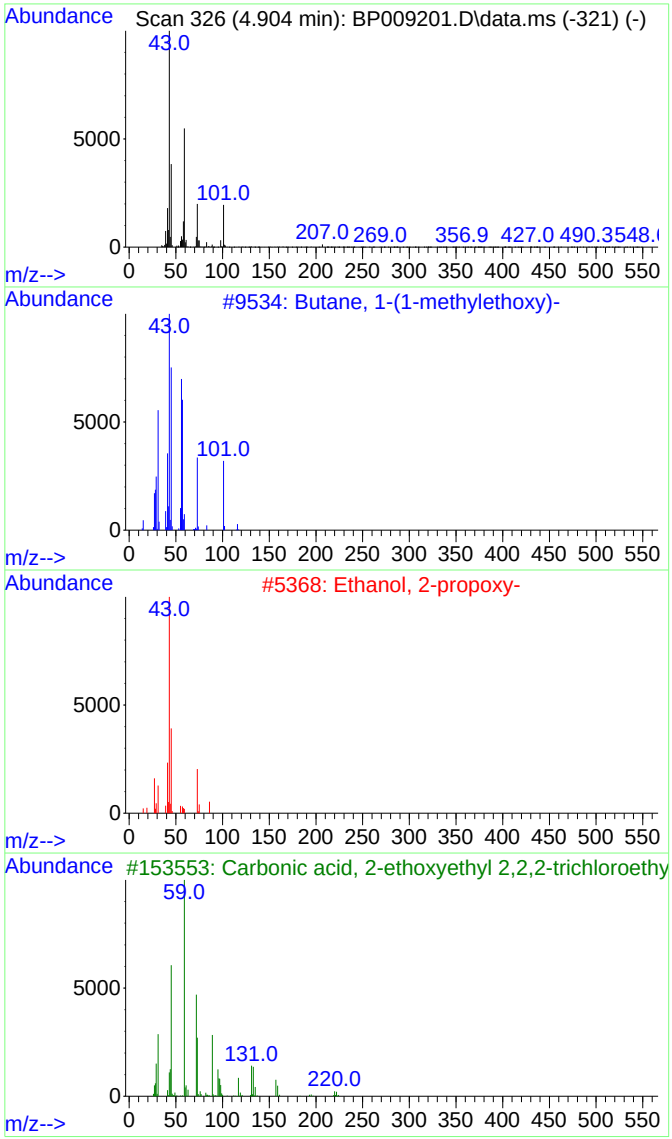
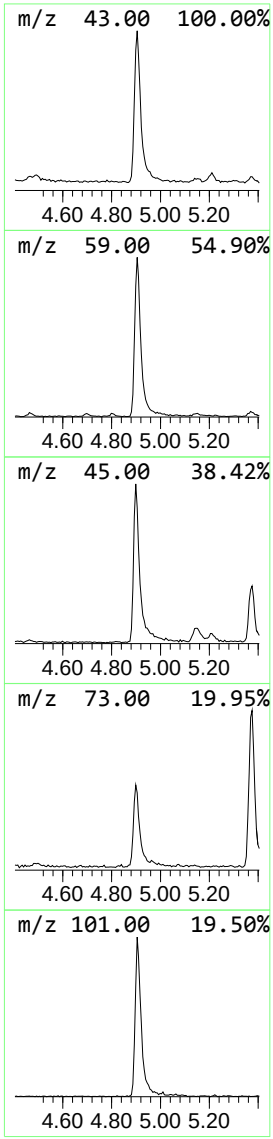
****

Peak Number 2 unknown4.904 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.904	3.13 ng	218886	1,4-Dichlorobenzene-d4	7.775

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 1-(1-methylethoxy)-	116	C7H16O	001860-27-1	47
2	Ethanol, 2-propoxy-	104	C5H12O2	002807-30-9	38
3	Carbonic acid, 2-ethoxyethyl 2,2...	264	C7H11Cl3O4	1000331-44-6	38
4	Silane, ethyldimethyl-	88	C4H12Si	000758-21-4	37
5	1-Propanol, 3,3'-oxybis-	134	C6H14O3	002396-61-4	37





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Data File : BP009201.D
Acq On : 17 Feb 2022 18:25
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Sample : N1575-07
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ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-15

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

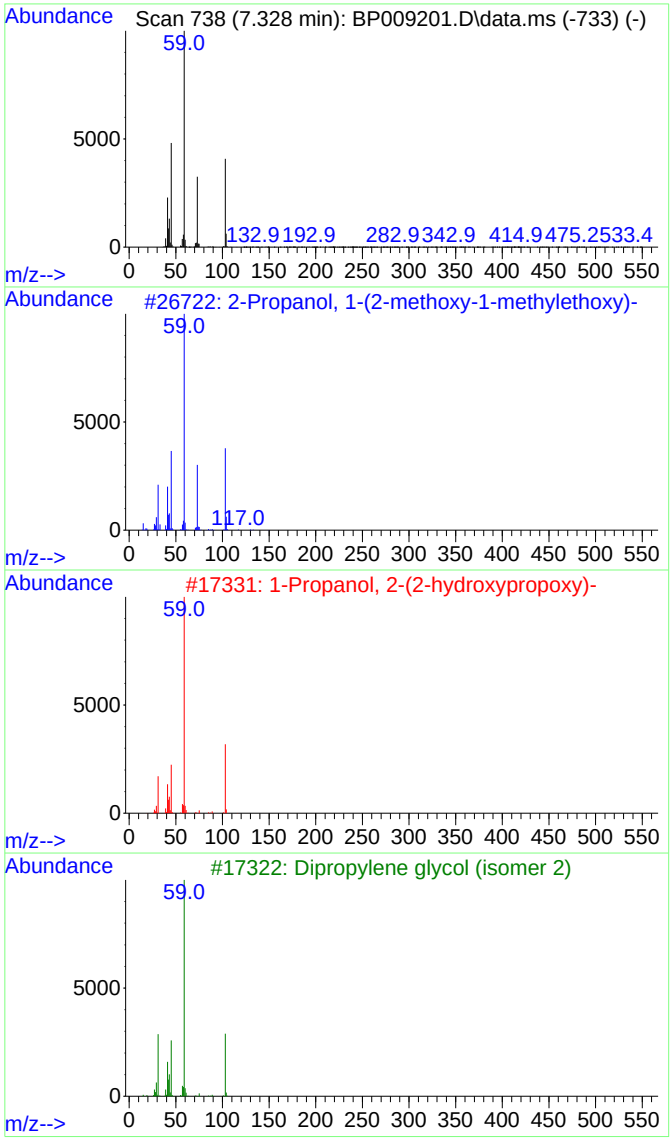
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

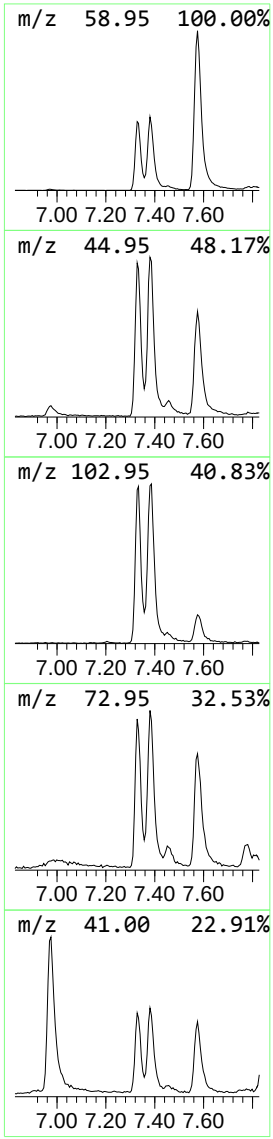
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.328	3.72 ng	260532	1,4-Dichlorobenzene-d4	7.775

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	90
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	53
3	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	53
4	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	50
5	2-Propanol, 1-(2-methoxypropoxy)-	148	C7H16O3	013429-07-7	47





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Sample : N1575-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-15

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

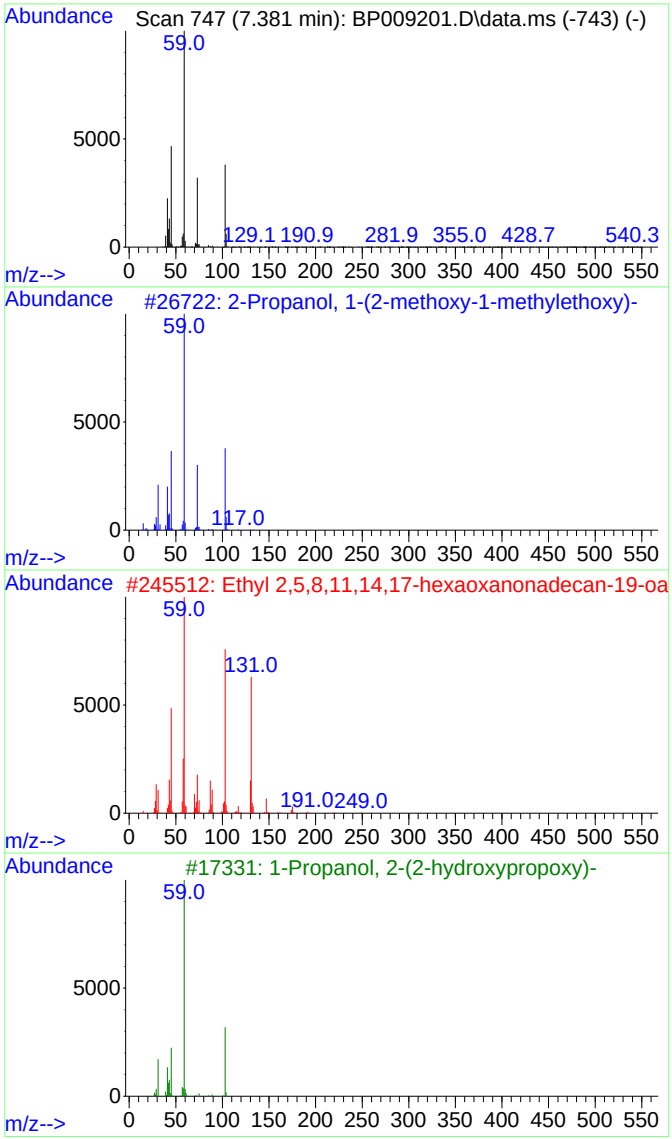
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

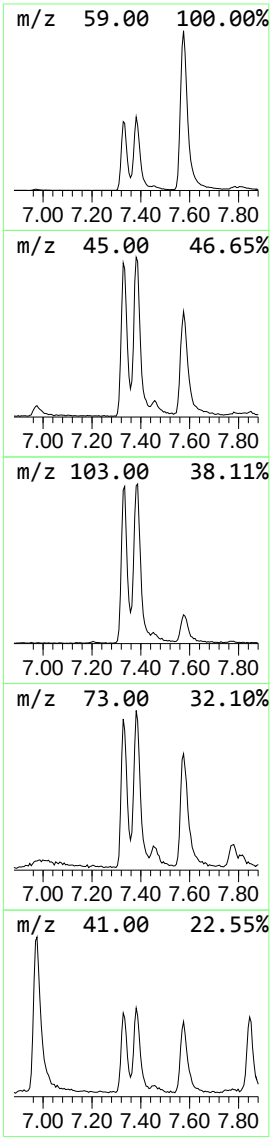
****

Peak Number 4 Ethyl 2,5,8,11,14,17-hexaox... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.381	4.11 ng	287437	1,4-Dichlorobenzene-d4	7.775

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	72
2	Ethyl 2,5,8,11,14,17-hexaoxanona...	338	C15H30O8	1000366-80-6	56
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	53
4	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	53
5	2-Propanol, 1-(2-ethoxypropoxy)-	162	C8H18O3	010143-32-5	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021722\
Data File : BP009201.D
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Operator : CG/JU
Sample : N1575-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-15

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

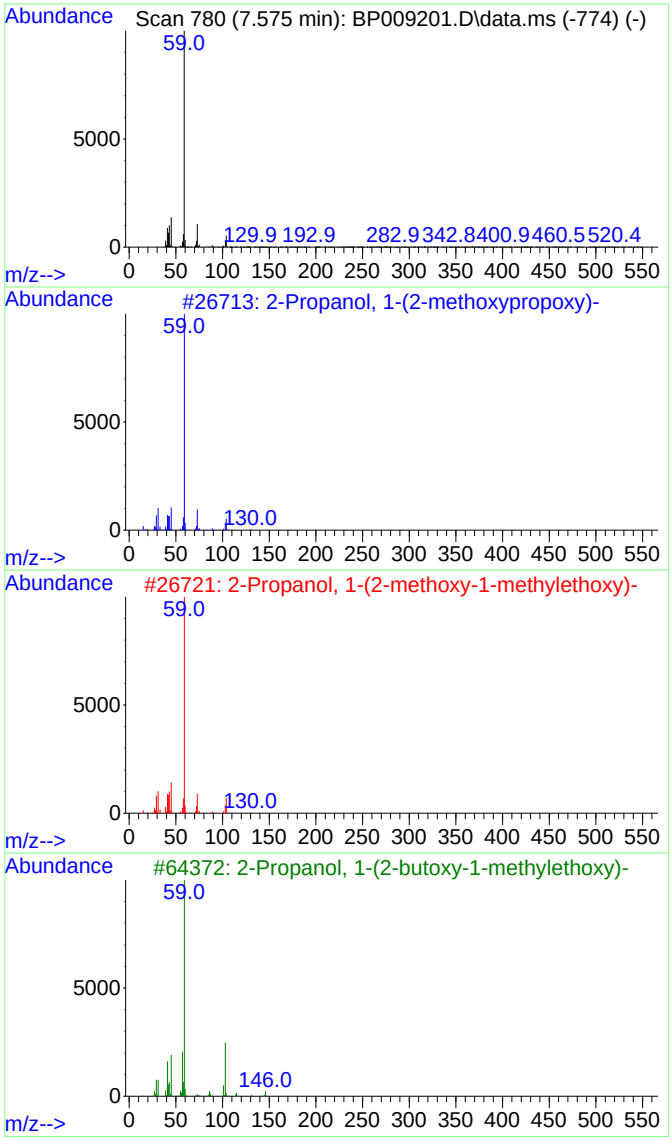
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

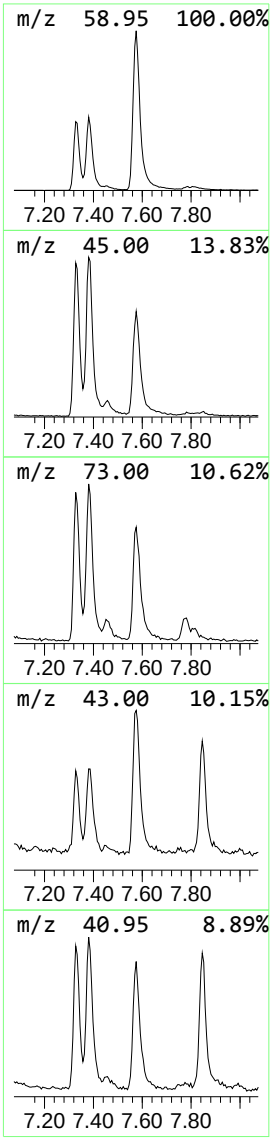
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.575	6.95 ng	486692	1,4-Dichlorobenzene-d4	7.775

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxypropoxy)-	148	C7H16O3	013429-07-7	83
2	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	83
3	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	64
4	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	64
5	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021722\
Data File : BP009201.D
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Operator : CG/JU
Sample : N1575-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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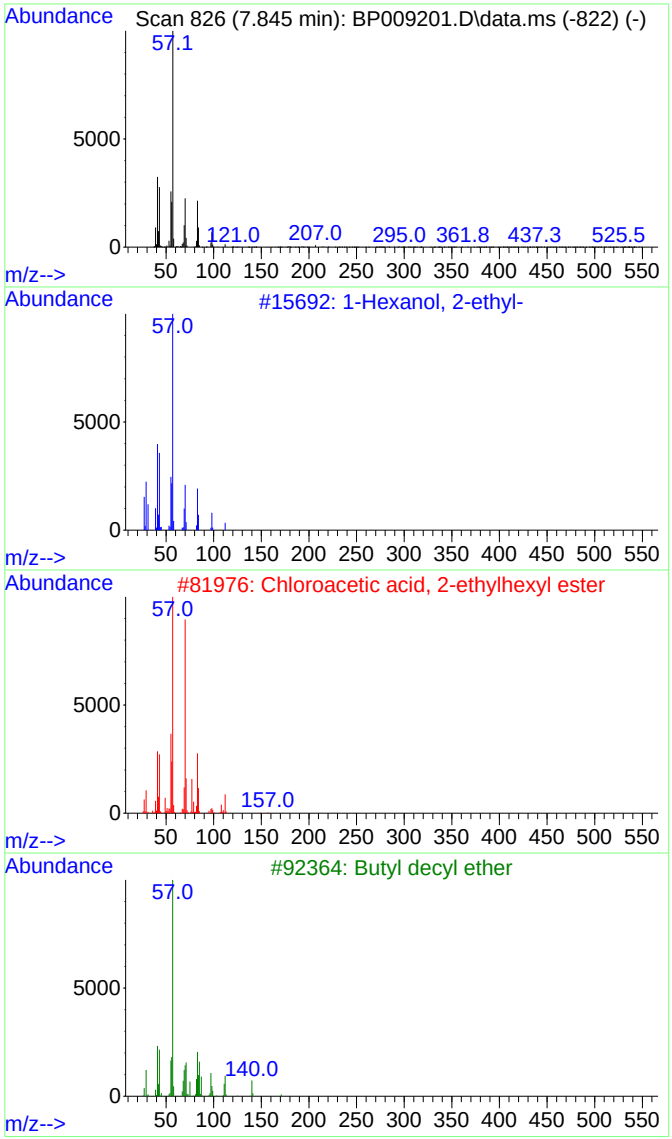
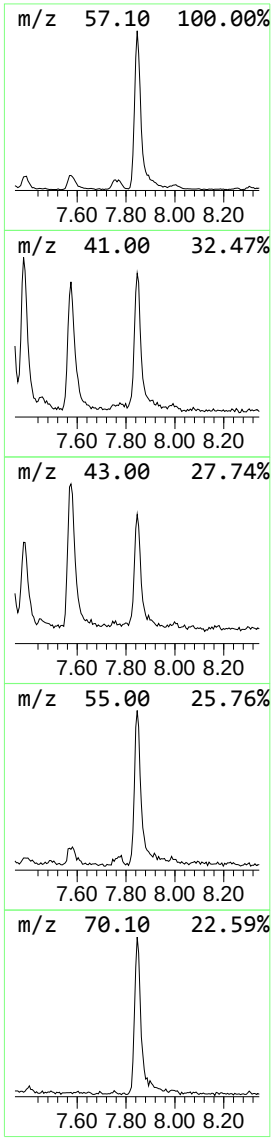
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.845	3.38 ng	236566	1,4-Dichlorobenzene-d4	7.775

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	Chloroacetic acid, 2-ethylhexyl ...	206	C10H19ClO2	005345-58-4	59
3	Butyl decyl ether	214	C14H30O	1000406-40-2	56
4	Isobutyl octan-2-yl carbonate	230	C13H26O3	1000372-74-7	56
5	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50





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Operator : CG/JU
Sample : N1575-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-15

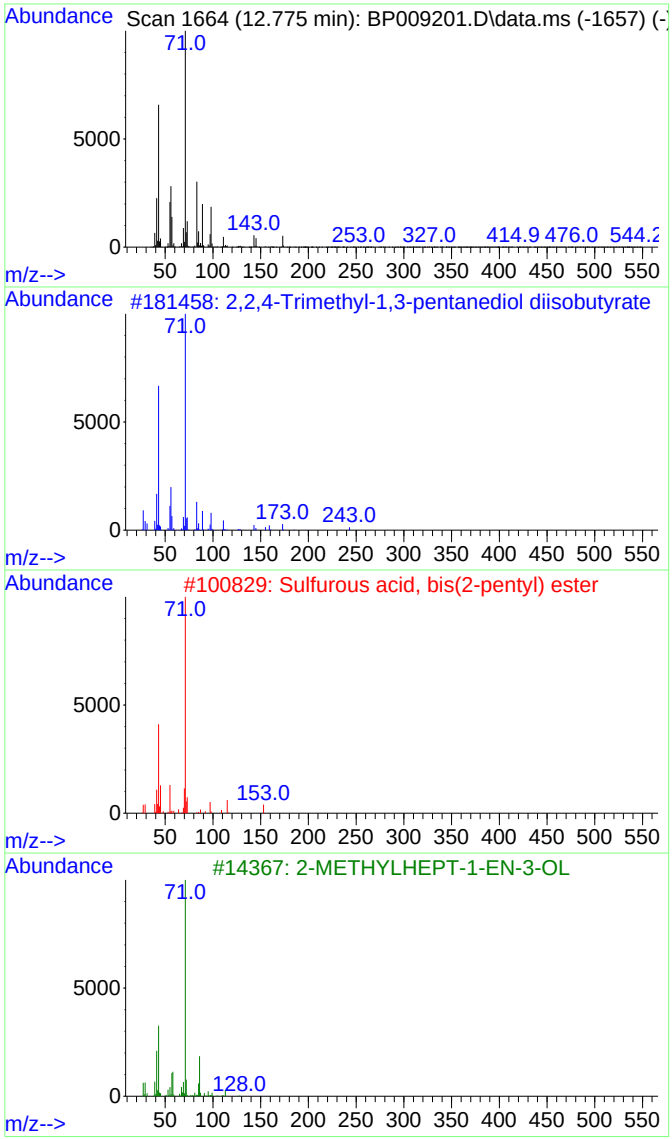
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

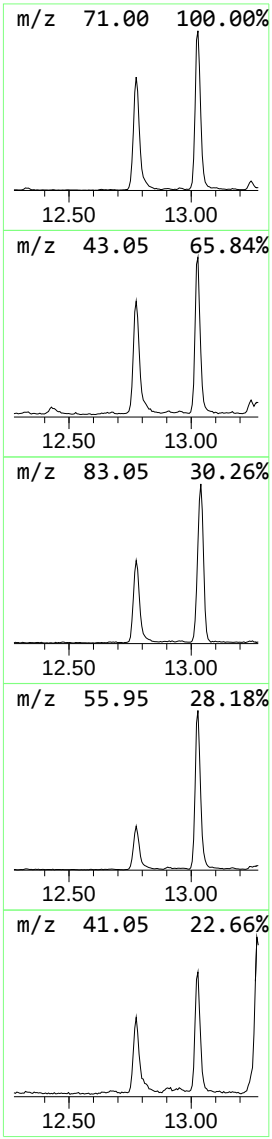
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 2,2,4-Trimethyl-1,3-pentane... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.775	2.93 ng	429664	Acenaphthene-d10	14.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	64
2	Sulfurous acid, bis(2-pentyl) ester	222	C10H22O3S	1000309-15-3	38
3	2-METHYLHEPT-1-EN-3-OL	128	C8H16O	013019-19-7	38
4	Butanoic acid, 2-butoxy-1-methyl...	216	C11H20O4	007492-70-8	38
5	3-Hexanone, 2,5-dimethyl-4-nitro-	173	C8H15NO3	059906-54-6	37





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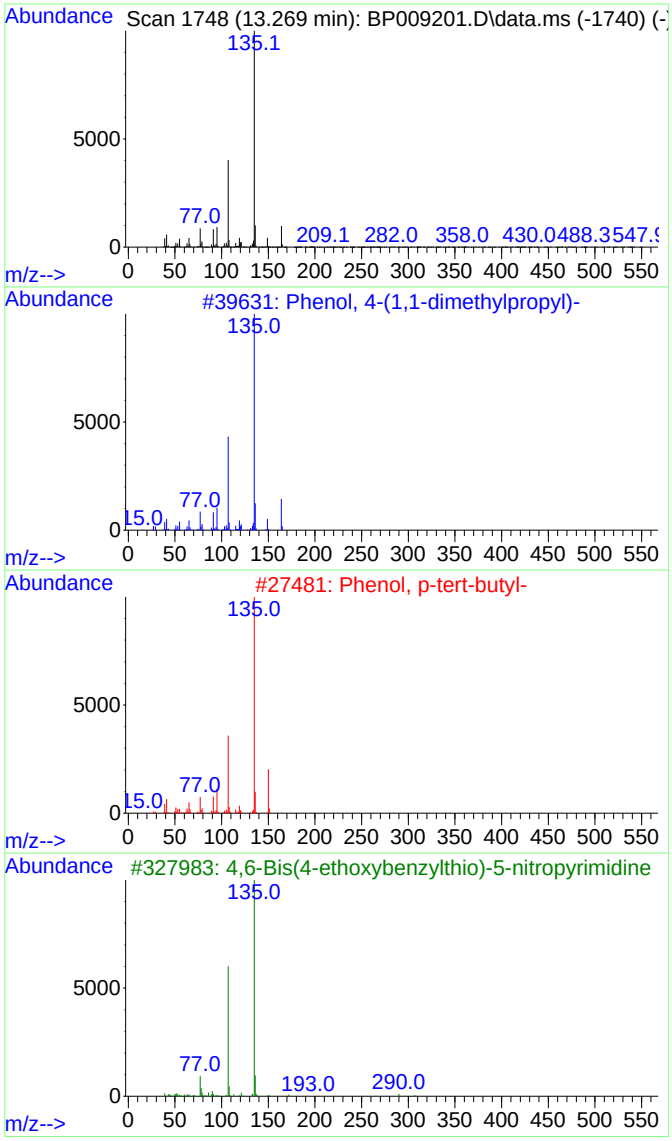
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

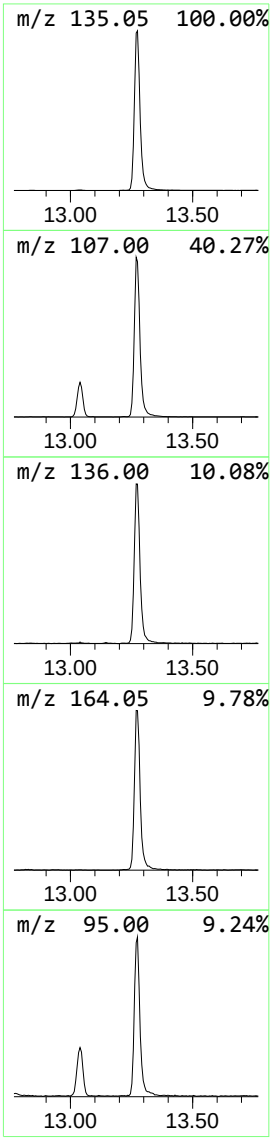
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Phenol, 4-(1,1-dimethylprop... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.269	13.07 ng	1917640	Acenaphthene-d10	14.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	96
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	80
3	4,6-Bis(4-ethoxybenzylthio)-5-ni...	457	C22H23N3O4S2	325957-76-4	64
4	4,4'-(1,2-diethylethylene)diphenol	270	C18H22O2	005635-50-7	64
5	Hexestrol, O-isopropyloxycarbonyl-	356	C22H28O4	1000487-68-4	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021722\
Data File : BP009201.D
Acq On : 17 Feb 2022 18:25
Operator : CG/JU
Sample : N1575-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-15

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.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	4.263	6.9	ng	485501	1	7.775	1400060	20.0
unknown4.904	4.904	3.1	ng	218886	1	7.775	1400060	20.0
2-Propanol, 1-(...	7.328	3.7	ng	260532	1	7.775	1400060	20.0
Ethyl 2,5,8,11,...	7.381	4.1	ng	287437	1	7.775	1400060	20.0
2-Propanol, 1-(...	7.575	7.0	ng	486692	1	7.775	1400060	20.0
1-Hexanol, 2-et...	7.845	3.4	ng	236566	1	7.775	1400060	20.0
2,2,4-Trimethyl...	12.775	2.9	ng	429664	3	14.416	2934710	20.0
Phenol, 4-(1,1-...	13.269	13.1	ng	1917640	3	14.416	2934710	20.0