LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072823\
Data File : BP016422.D
Acq On : 28 Jul 2023 14:30
Operator : MA/JU
Sample : 03630-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SP-303-20230713

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-BP072723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP016422.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.605	386	394	403	rBV	3840112	5773430	18.67%	4.578%
2	5.916	441	447	453	rBV	590812	942640	3.05%	0.747%
3	6.011	457	463	473	rVB	1083489	1690712	5.47%	1.341%
4	6.722	577	584	598	rVB	650545	1028618	3.33%	0.816%
5	7.222	661	669	682	rBV	2466559	3807680	12.31%	3.019%
6	8.087	809	816	828	rBV	1671672	2730881	8.83%	2.165%
7	8.358	857	862	868	rBV	195562	331157	1.07%	0.263%
8	8.428	868	874	884	rVB	959142	1523444	4.93%	1.208%
9	9.287	1010	1020	1029	rBV	5795453	9553613	30.90%	7.575%
10	10.557	1230	1236	1250	rVB	435707	869621	2.81%	0.690%
11	10.922	1290	1298	1306	rBV	2358037	3936698	12.73%	3.121%
12	13.363	1705	1713	1719	rBV	13701506	21031724	68.02%	16.677%
13	14.734	1938	1946	1955	rBV	3622770	5242803	16.96%	4.157%
14	16.228	2192	2200	2217	rBV	9622775	14781362	47.81%	11.720%
15	17.498	2409	2416	2426	rBV	4576453	6584722	21.30%	5.221%
16	20.039	2842	2848	2854	rBV	22338688	30919171	100.00%	24.517%
17	21.586	3105	3111	3122	rBV	5759508	7509498	24.29%	5.954%
18	24.186	3544	3553	3564	rBV	3661399	7857933	25.41%	6.231%

Sum of corrected areas: 126115707

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072823\
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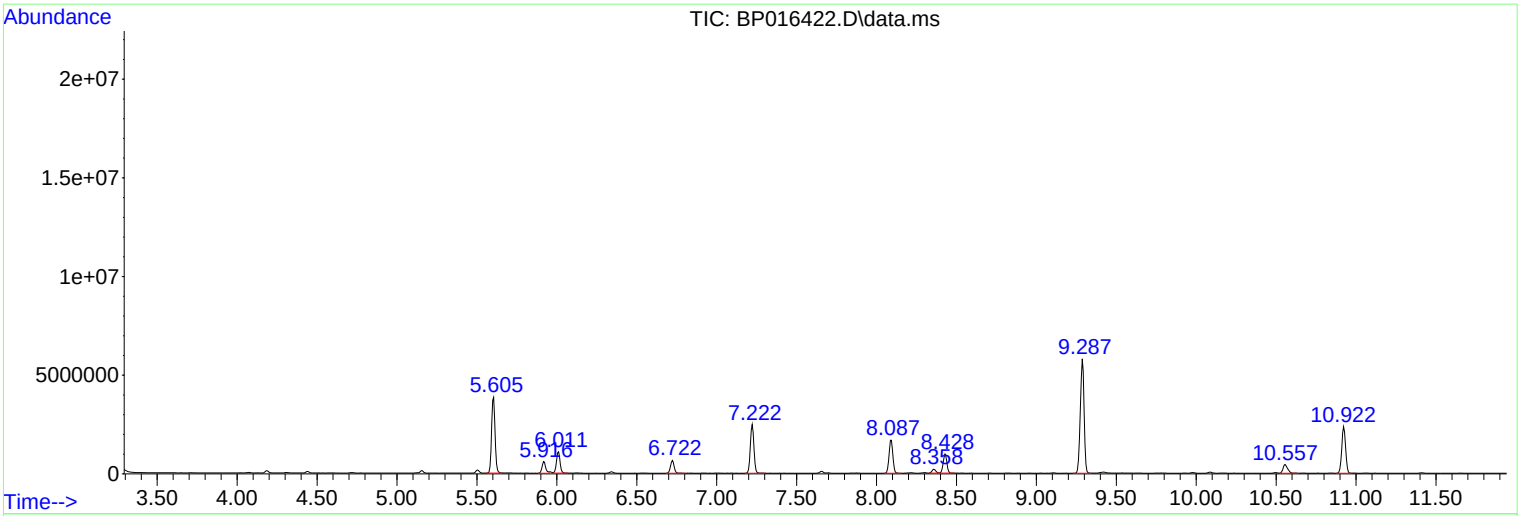
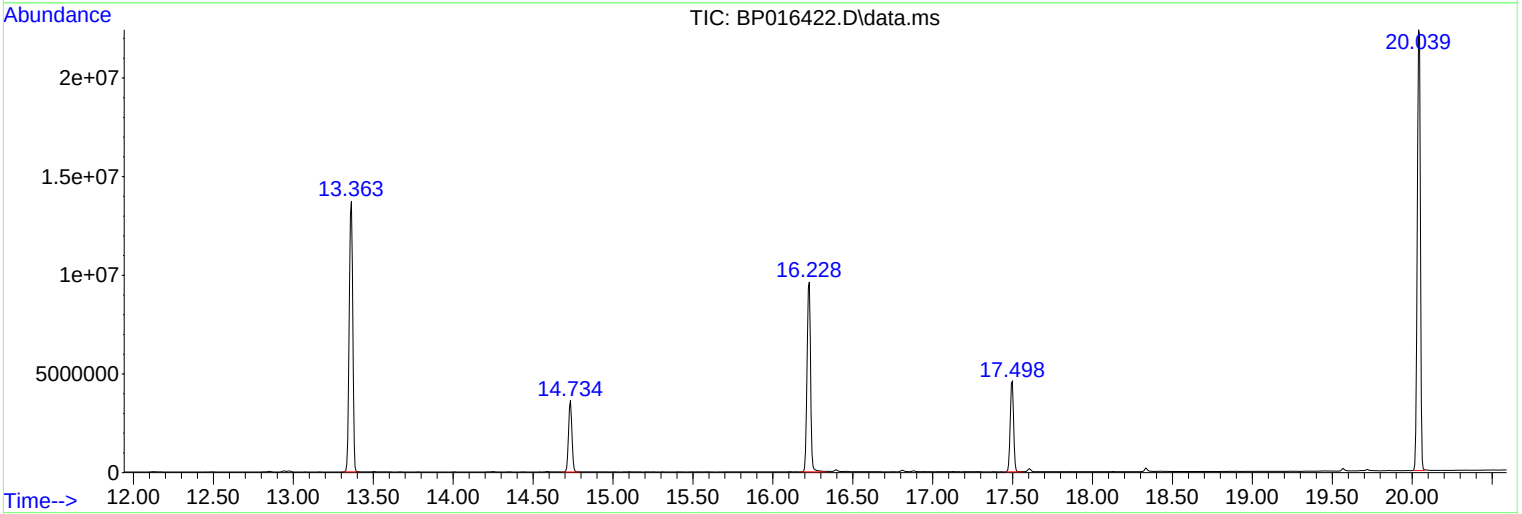
Misc :
ALS Vial : 13 Sample Multiplier: 1

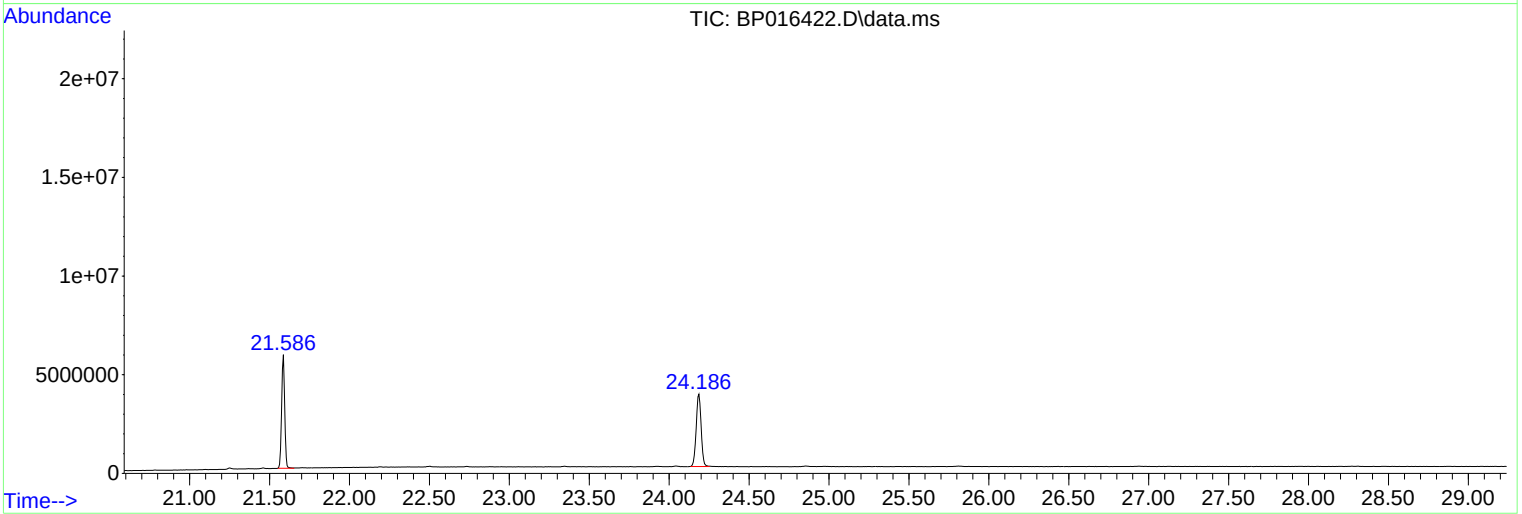
Instrument :
BNA_P
ClientSampleId :
SP-303-20230713

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP072723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072823\
Data File : BP016422.D
Acq On : 28 Jul 2023 14:30
Operator : MA/JU
Sample : 03630-03
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BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP072723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

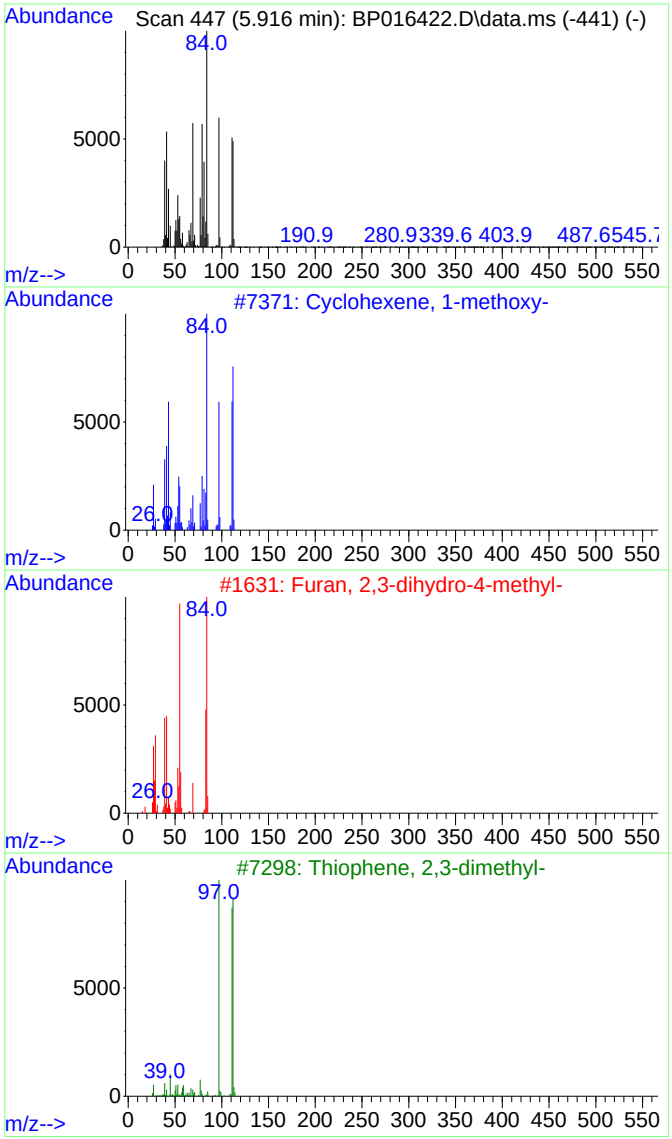
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

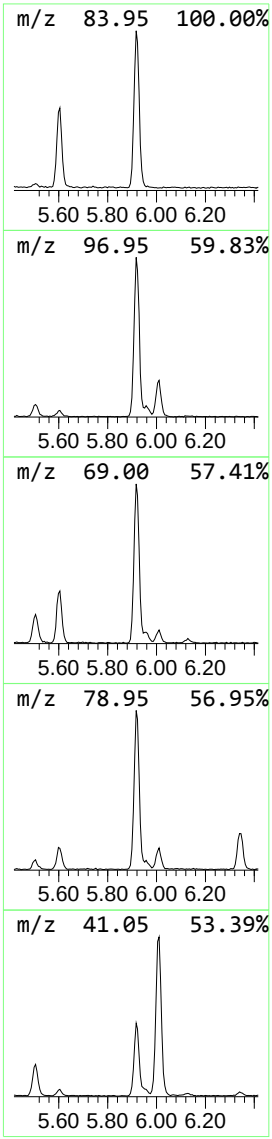
****

Peak Number 1 unknown5.916 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.916	6.90 ng	942640	1,4-Dichlorobenzene-d4	8.093

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene, 1-methoxy-	112	C7H12O	000931-57-7	27
2	Furan, 2,3-dihydro-4-methyl-	84	C5H8O	034314-83-5	27
3	Thiophene, 2,3-dimethyl-	112	C6H8S	000632-16-6	25
4	1-Hepten-6-yne	94	C7H10	065939-59-5	25
5	2-Cyclohexen-1-one, 4-hydroxy-	112	C6H8O2	030182-12-8	25





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Data File : BP016422.D
Acq On : 28 Jul 2023 14:30
Operator : MA/JU
Sample : 03630-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SP-303-20230713

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP072723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

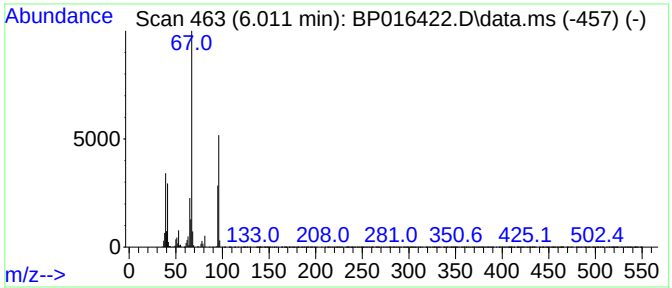
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

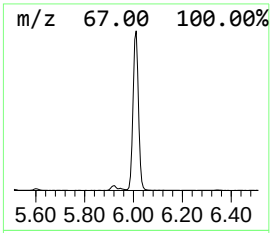
****

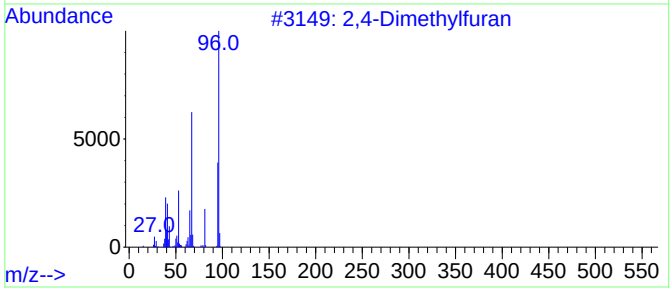
Peak Number 2 2,4-Dimethylfuran Concentration Rank 1

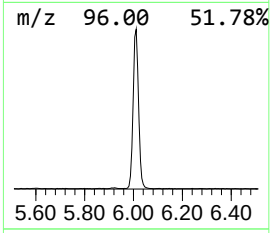
R.T.	EstConc	Area	Relative to ISTD	R.T.
6.011	12.38 ng	1690710	1,4-Dichlorobenzene-d4	8.093

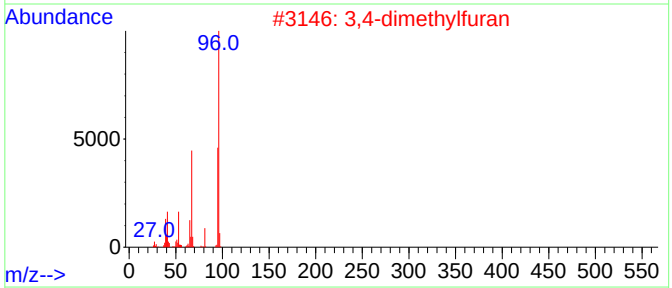
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Dimethylfuran	96	C6H8O	003710-43-8	91
2	3,4-dimethylfuran	96	C6H8O	1000458-50-4	78
3	2,3-dimethylfuran	96	C6H8O	1000458-49-9	53
4	Cyclobutane, 1-ethyl-3-methylene-	96	C7H12	056335-70-7	53
5	2-Cyclopenten-1-one, 2-methyl-	96	C6H8O	001120-73-6	43

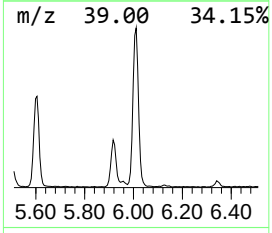


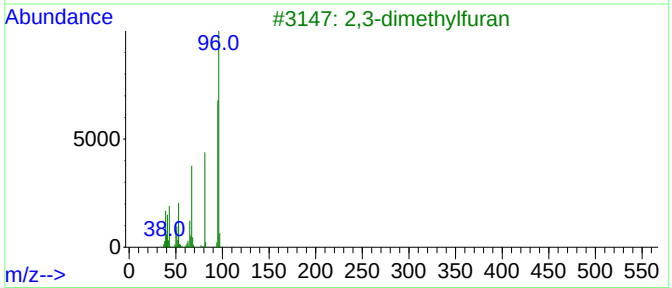


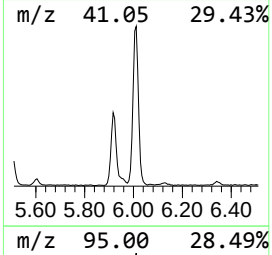


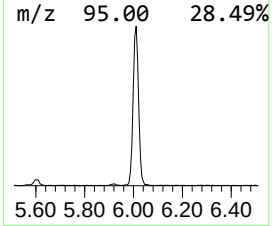












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Data File : BP016422.D
Acq On : 28 Jul 2023 14:30
Operator : MA/JU
Sample : 03630-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SP-303-20230713

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP072723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

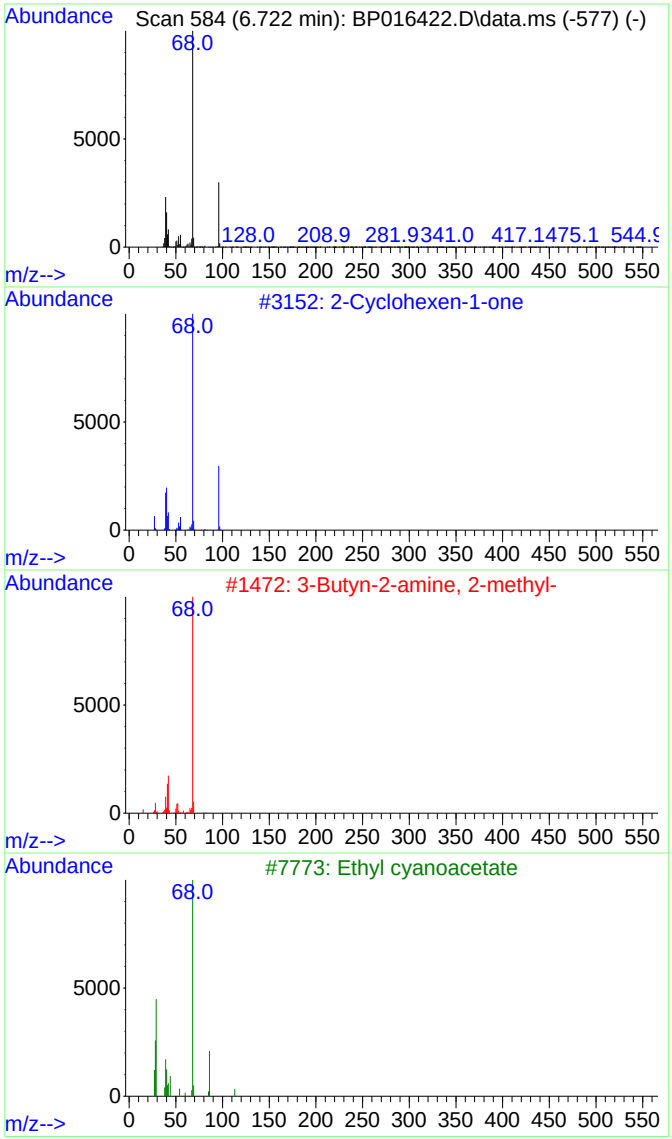
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

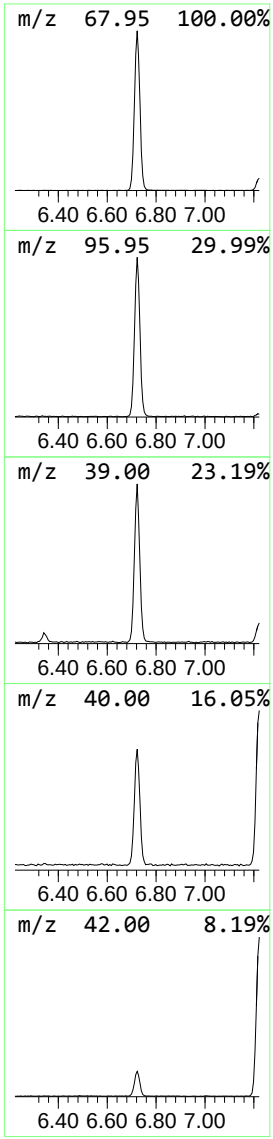
****

Peak Number 3 2-Cyclohexen-1-one Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.722	7.53 ng	1028620	1,4-Dichlorobenzene-d4	8.093

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	91
2	3-Butyn-2-amine, 2-methyl-	83	C5H9N	002978-58-7	42
3	Ethyl cyanoacetate	113	C5H7NO2	000105-56-6	36
4	2,5-Dihydro-3-methyl-thiophene 1...	132	C5H8O2S	001193-10-8	12
5	1H-Imidazole	68	C3H4N2	000288-32-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072823\
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

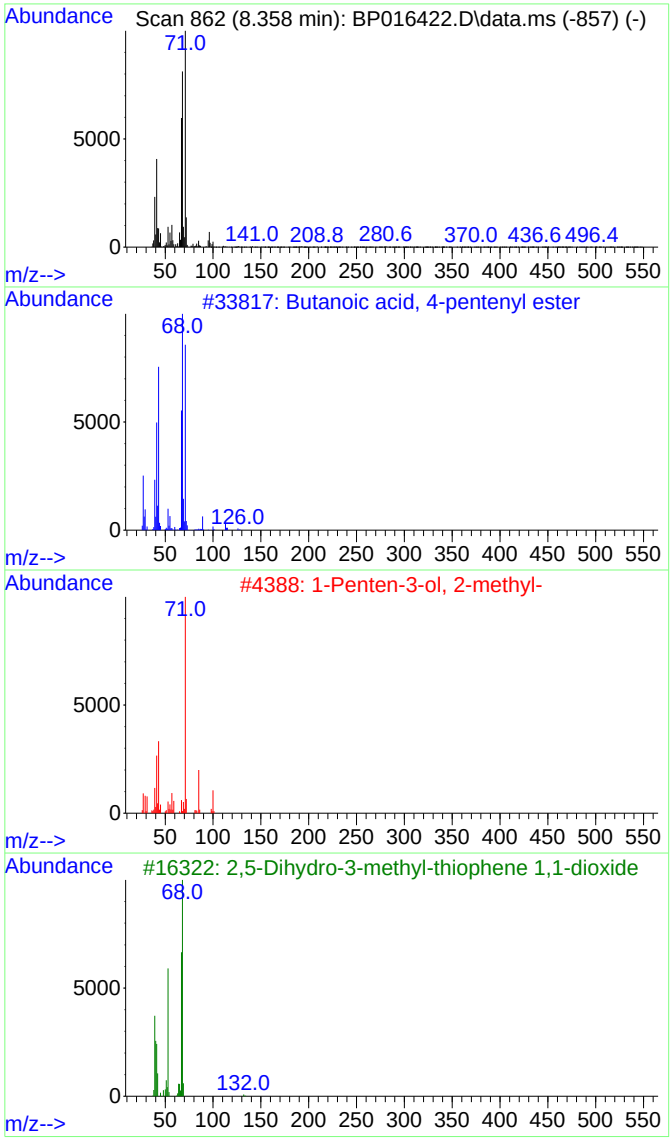
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

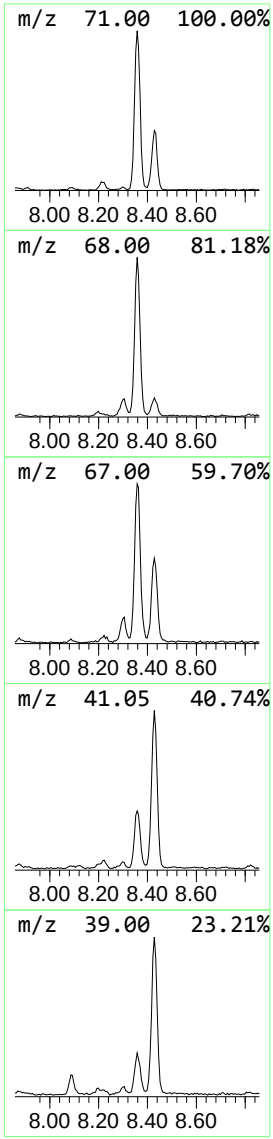
****

Peak Number 4 Butanoic acid, 4-pentenyl e... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.358	2.43 ng	331157	1,4-Dichlorobenzene-d4	8.093

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 4-pentenyl ester	156	C9H16O2	030563-31-6	56
2	1-Penten-3-ol, 2-methyl-	100	C6H12O	002088-07-5	38
3	2,5-Dihydro-3-methyl-thiophene 1...	132	C5H8O2S	001193-10-8	32
4	Pent-4-en-1-yl propyl carbonate	172	C9H16O3	1000372-91-0	32
5	Cyclopentanemethanol	100	C6H12O	003637-61-4	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072823\
Data File : BP016422.D
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Operator : MA/JU
Sample : 03630-03
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ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP072723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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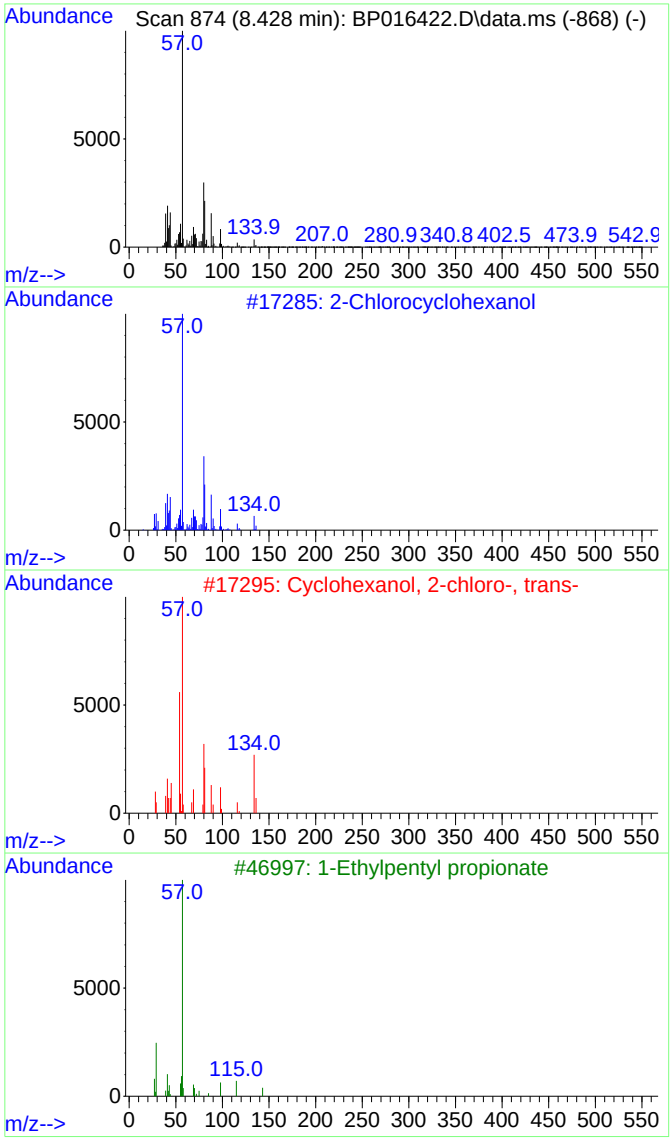
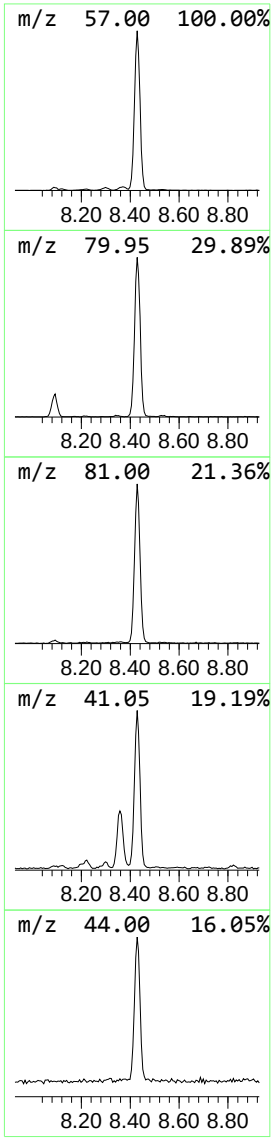
****

Peak Number 5 2-Chlorocyclohexanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.428	11.16 ng	1523440	1,4-Dichlorobenzene-d4	8.093

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Chlorocyclohexanol	134	C6H11ClO	001561-86-0	95
2	Cyclohexanol, 2-chloro-, trans-	134	C6H11ClO	006628-80-4	50
3	1-Ethylpentyl propionate	172	C10H20O2	1000430-89-7	25
4	Oxalic acid, isobutyl heptyl ester	244	C13H24O4	1000309-37-2	22
5	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	17





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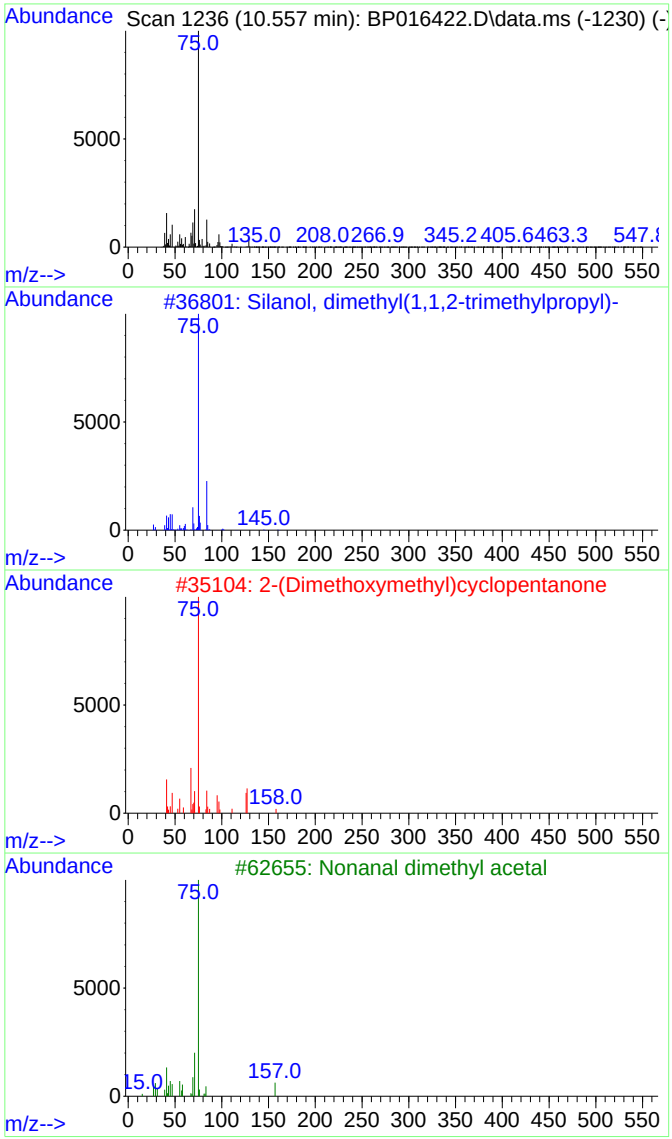
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

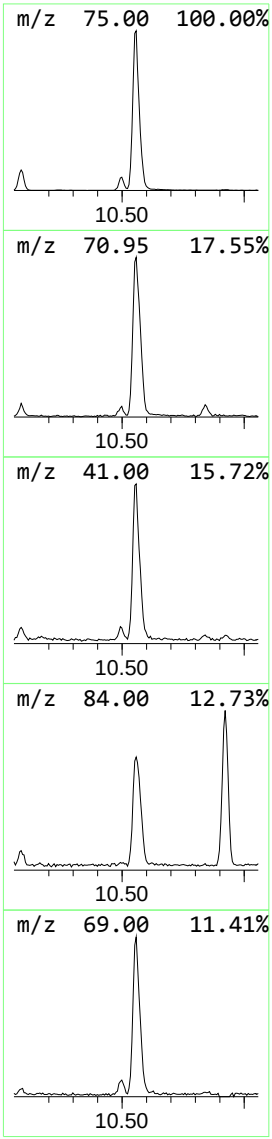
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Silanol, dimethyl(1,1,2-tri... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.557	4.42 ng	869621	Naphthalene-d8	10.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Silanol, dimethyl(1,1,2-trimethy...	160	C8H20OSi	055644-10-5	64
2	2-(Dimethoxymethyl)cyclopentanone	158	C8H14O3	1000424-64-6	64
3	Nonanal dimethyl acetal	188	C11H24O2	018824-63-0	59
4	Dodecane, 1,1-dimethoxy-	230	C14H30O2	014620-52-1	59
5	Heptane, 1,1-dimethoxy-	160	C9H20O2	010032-05-0	50





Tentatively Identified Compound (LSC) summary

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown5.916	5.916	6.9	ng	942640	1	8.093	2730880	20.0
2,4-Dimethylfuran	6.011	12.4	ng	1690710	1	8.093	2730880	20.0
2-Cyclohexen-1-one	6.722	7.5	ng	1028620	1	8.093	2730880	20.0
Butanoic acid, ...	8.358	2.4	ng	331157	1	8.093	2730880	20.0
2-Chlorocyclohe...	8.428	11.2	ng	1523440	1	8.093	2730880	20.0
Silanol, dimeth...	10.557	4.4	ng	869621	2	10.922	3936700	20.0