

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071024\
 Data File : BF138500.D
 Acq On : 10 Jul 2024 14:29
 Operator : CG\JU
 Sample : PB161976BL
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB161976BL

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-BF070924.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138500.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.275	3	32	38	rVB	1063844	3870353	98.74%	14.256%
2	4.216	360	362	375	rBV	24551	60131	1.53%	0.221%
3	5.104	506	513	521	rBV	1408058	1818232	46.39%	6.697%
4	5.498	576	580	584	rBV	2327320	2154683	54.97%	7.937%
5	5.669	606	609	619	rVB2	128946	135051	3.45%	0.497%
6	6.116	681	685	688	rBV	240829	195037	4.98%	0.718%
7	6.498	745	750	753	rBV	2431727	2266395	57.82%	8.348%
8	6.863	808	812	815	rBV	844153	643353	16.41%	2.370%
9	6.963	824	829	834	rBV	44011	45236	1.15%	0.167%
10	7.016	834	838	842	rBV	224620	210117	5.36%	0.774%
11	7.428	902	908	911	rBV	2127425	2220218	56.64%	8.178%
12	7.775	963	967	971	rBV	41055	40593	1.04%	0.150%
13	8.145	1025	1030	1033	rBV	971636	868323	22.15%	3.198%
14	9.222	1207	1213	1216	rBV	4039461	3806846	97.12%	14.022%
15	9.898	1322	1328	1331	rBV	1194928	981318	25.04%	3.615%
16	10.686	1458	1462	1465	rBV	1655980	1429192	36.46%	5.264%
17	11.386	1577	1581	1584	rBV	1180886	1060179	27.05%	3.905%
18	12.974	1845	1851	1854	rBV	4144206	3919696	100.00%	14.438%
19	14.021	2025	2029	2032	rBV	806061	729081	18.60%	2.686%
20	15.486	2272	2278	2287	rBV	410744	559625	14.28%	2.061%
21	15.945	2351	2356	2365	rBV2	26551	40152	1.02%	0.148%
22	16.451	2437	2442	2451	rVB2	26675	52725	1.35%	0.194%
23	17.051	2538	2544	2553	rVB2	19942	41775	1.07%	0.154%

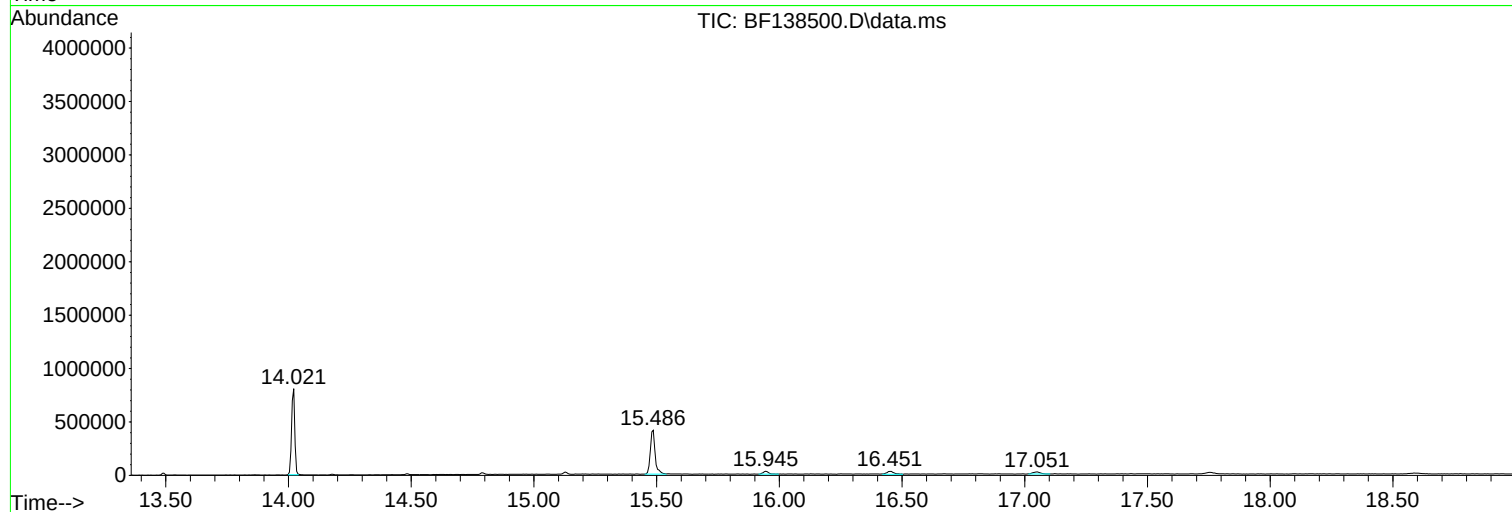
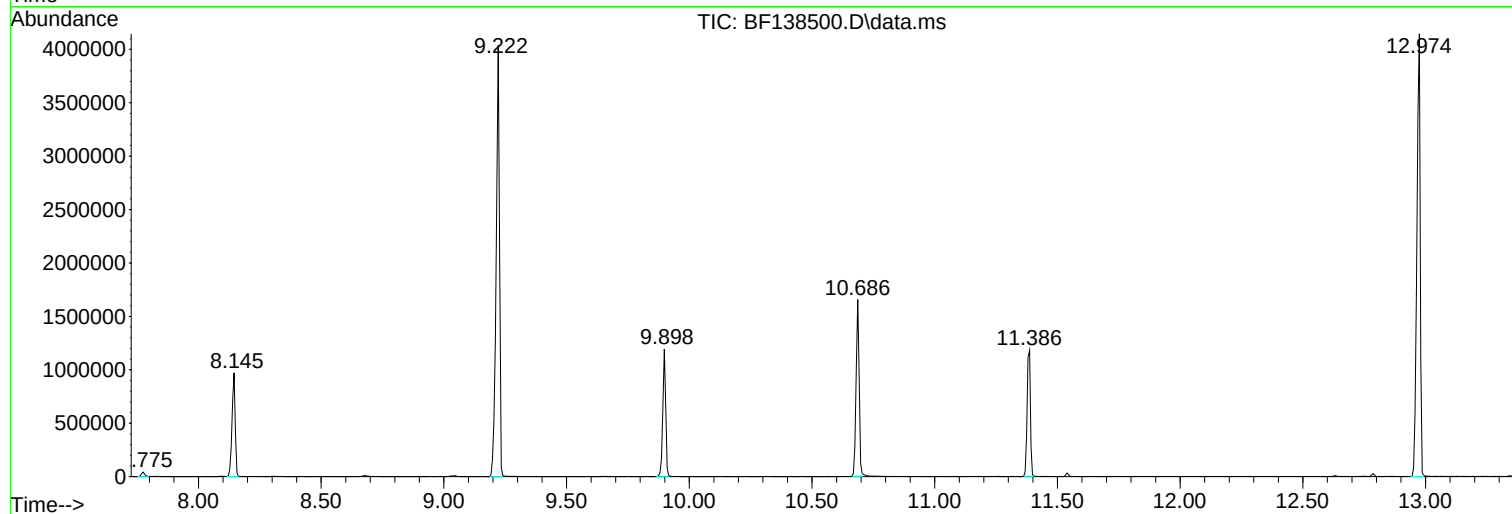
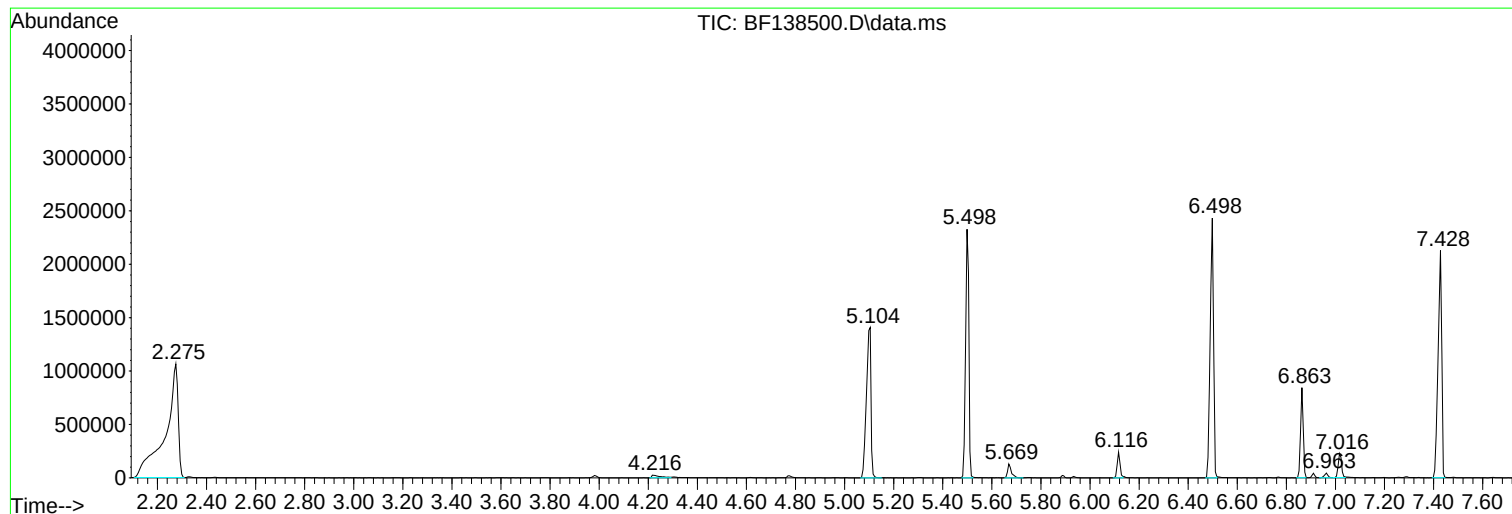
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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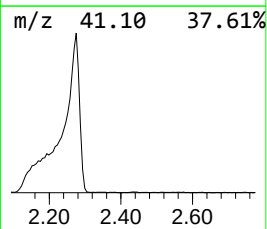
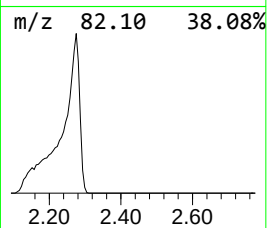
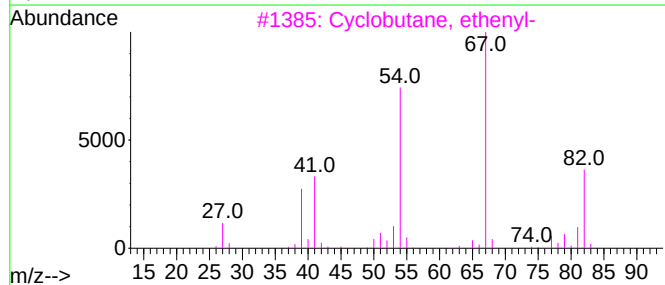
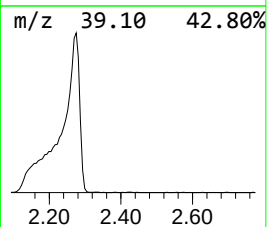
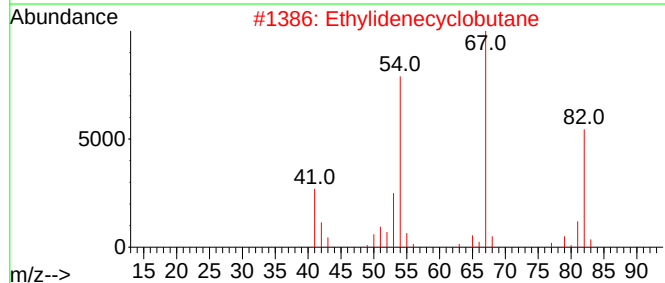
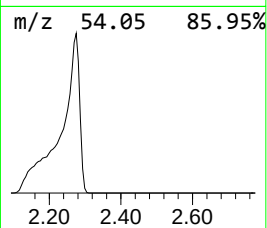
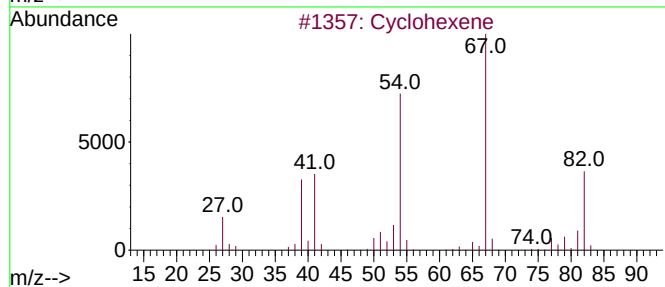
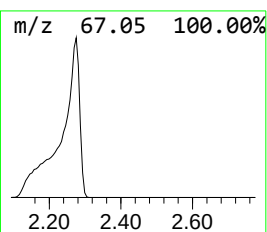
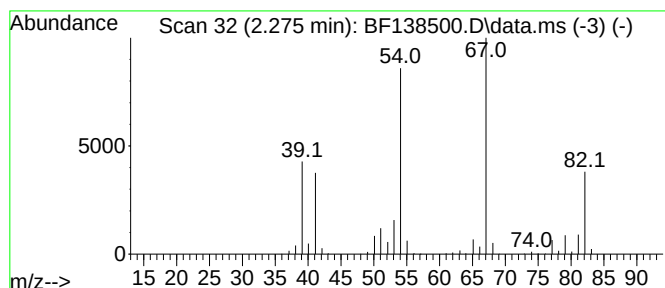
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Cyclohexene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.275	120.32 ng	3870350	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexene	82	C6H10	000110-83-8	93
2			Ethylidenecyclobutane	82	C6H10	001528-21-8	91
3			Cyclobutane, ethenyl-	82	C6H10	002597-49-1	90
4			C2H5CH=CHCH=CH2	82	C6H10	000592-48-3	42
5			1,3-Pentadiene, 2-methyl-	82	C6H10	001118-58-7	38



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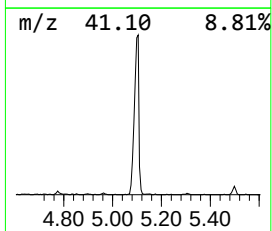
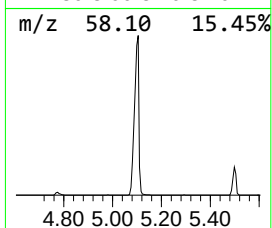
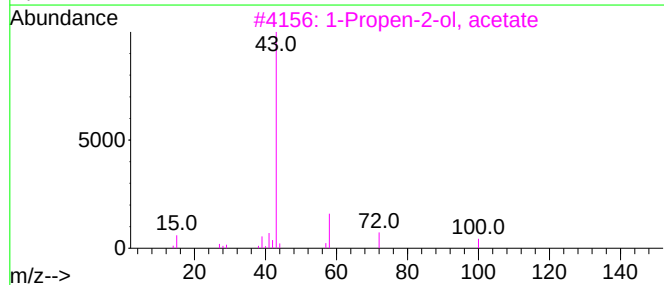
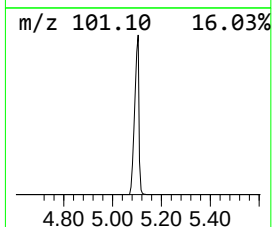
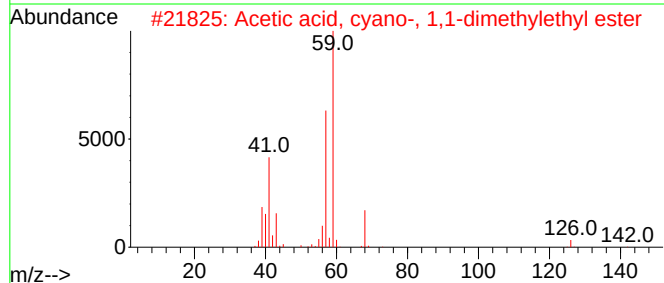
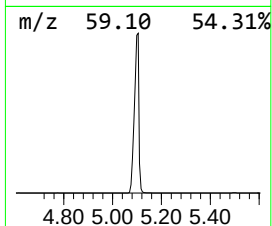
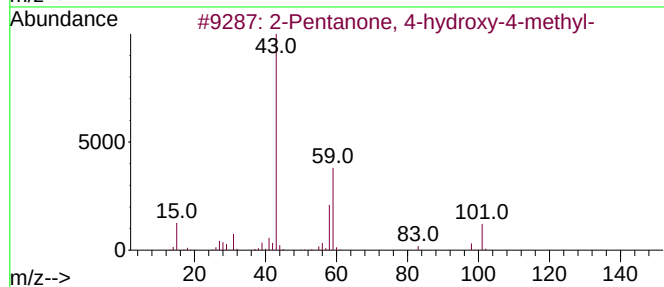
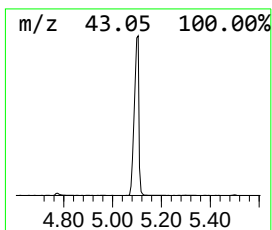
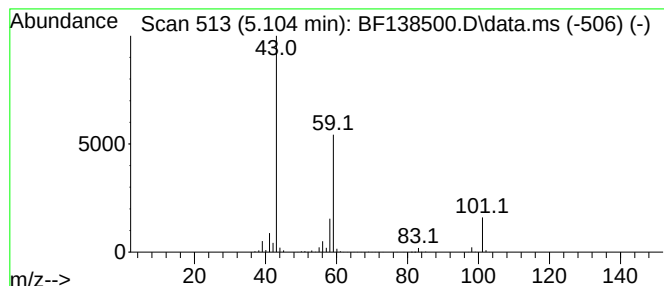
Instrument :
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ClientSampleId :
PB161976BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.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-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.104	56.52 ng	1818230	1,4-Dichlorobenzene-d4	6.863	
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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9



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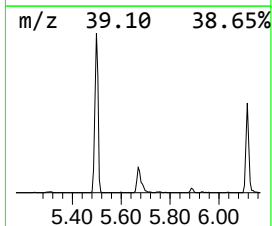
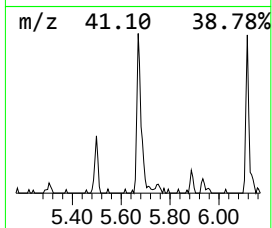
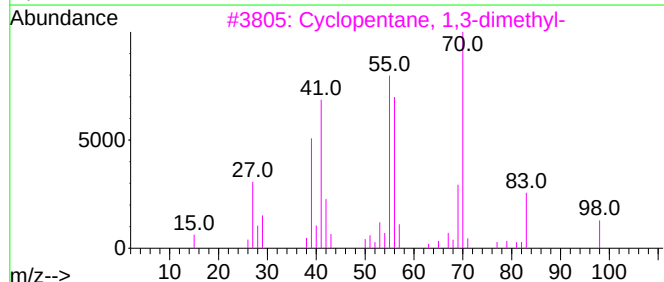
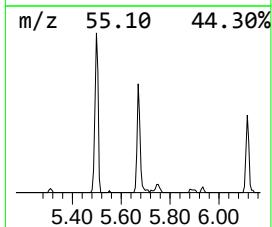
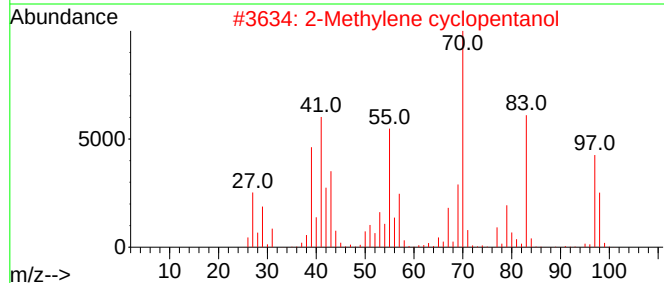
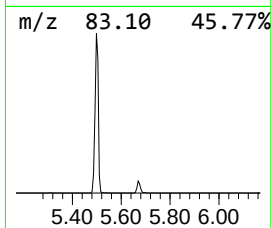
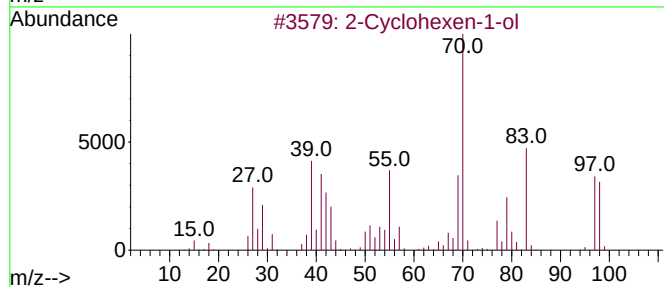
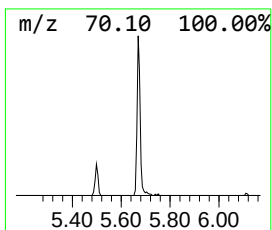
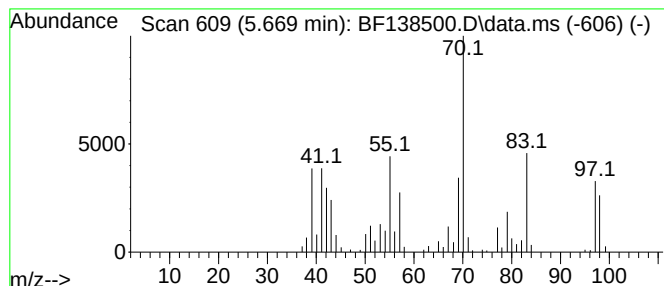
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BNA_F
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PB161976BL

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TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Cyclohexen-1-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.669	4.20 ng	135051	1,4-Dichlorobenzene-d4			6.863
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-ol		98	C6H10O	000822-67-3	94
2	2-Methylene cyclopentanol		98	C6H10O	020461-31-8	58
3	Cyclopentane, 1,3-dimethyl-		98	C7H14	002453-00-1	47
4	Cyclopentane, 1,3-dimethyl-, cis-		98	C7H14	002532-58-3	38
5	2,6-Cyclooctadien-1-ol		124	C8H12O	010017-18-2	35



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ClientSampleId :
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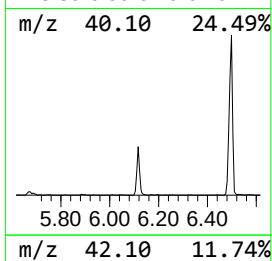
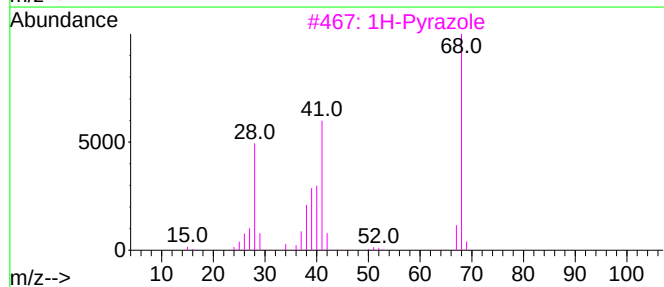
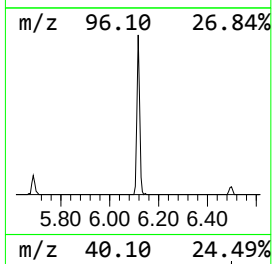
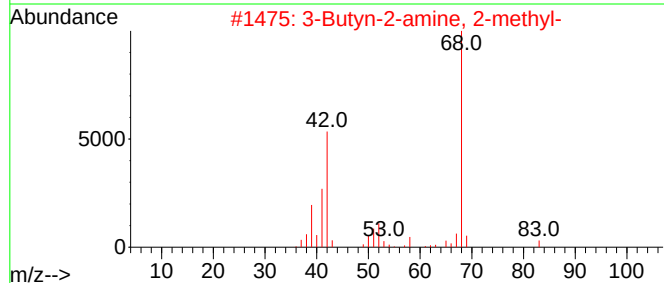
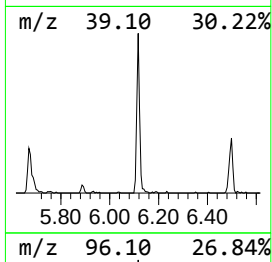
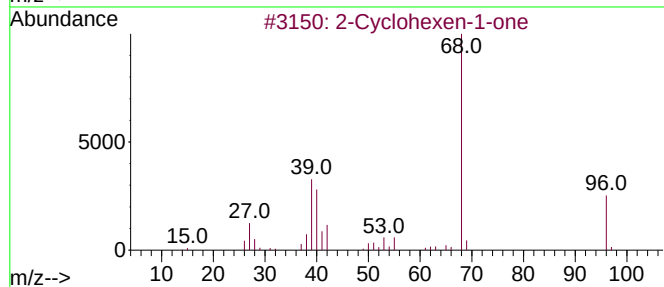
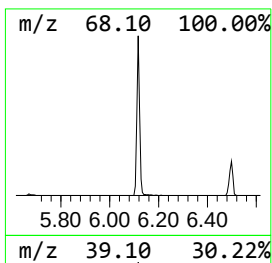
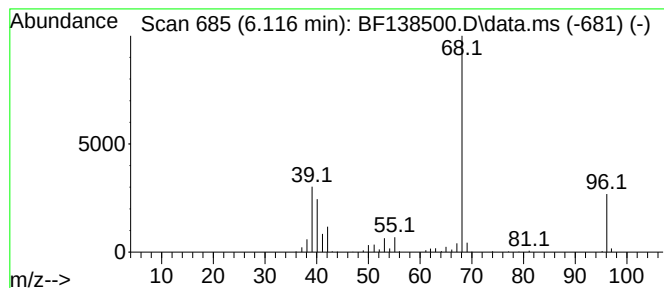
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 2-Cyclohexen-1-one Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.116	6.06 ng	195037	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Cyclohexen-1-one	96	C6H8O	000930-68-7	94
2			3-Butyn-2-amine, 2-methyl-	83	C5H9N	002978-58-7	45
3			1H-Pyrazole	68	C3H4N2	000288-13-1	36
4			2,5-Dihydro-3-methyl-thiophene 1...	132	C5H8O2S	001193-10-8	33
5			But-1-ene-3-yne, 1-ethoxy-	96	C6H8O	002806-41-9	14



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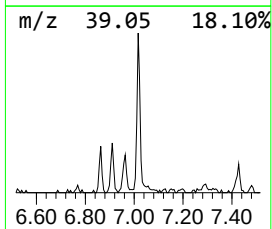
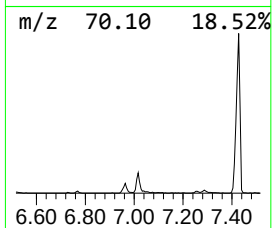
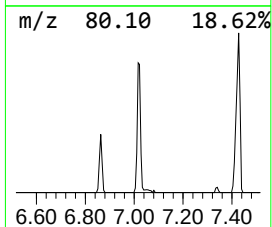
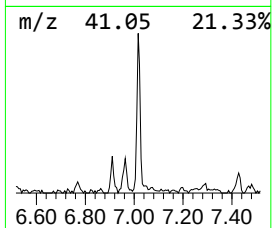
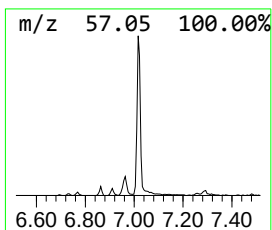
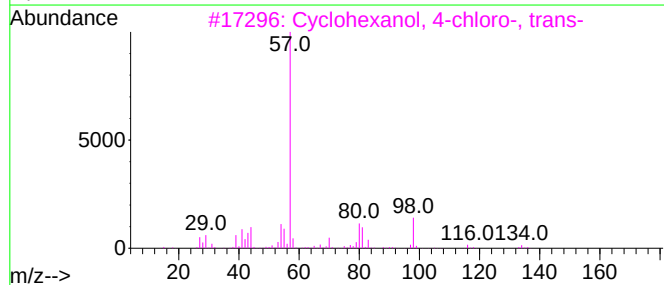
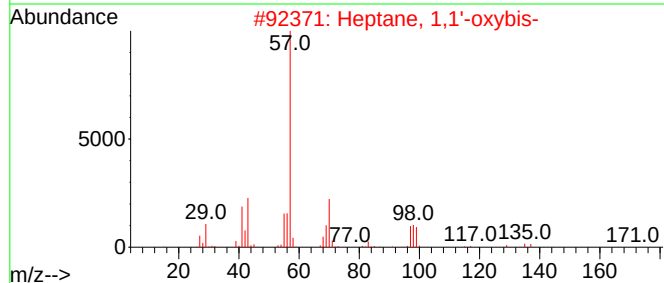
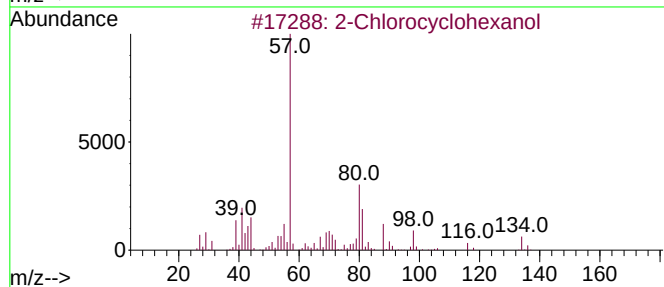
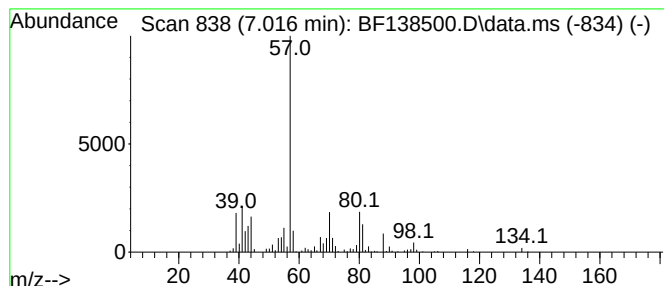
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 2-Chlorocyclohexanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.016	6.53 ng	210117	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Chlorocyclohexanol	134	C6H11ClO	001561-86-0	64
2			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	38
3			Cyclohexanol, 4-chloro-, trans-	134	C6H11ClO	029538-77-0	38
4			3-Furanol, tetrahydro-	88	C4H8O2	000453-20-3	38
5			Cyclohexanol, 2-chloro-, trans-	134	C6H11ClO	006628-80-4	30



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclohexene	2.275	120.3	ng	3870350	1	6.863	643353	20.0
2-Pentanone, 4-...	5.104	56.5	ng	1818230	1	6.863	643353	20.0
2-Cyclohexen-1-ol	5.669	4.2	ng	135051	1	6.863	643353	20.0
2-Cyclohexen-1-one	6.116	6.1	ng	195037	1	6.863	643353	20.0
2-Chlorocyclohe...	7.016	6.5	ng	210117	1	6.863	643353	20.0