LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071023\
Data File : BF134191.D
Acq On : 10 Jul 2023 17:50
Operator : CG\JU
Sample : PB153729BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB153729BL

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-BF062623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134191.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.234	3	25	34	rVB	1113464	4301562	100.00%	16.148%
2	5.093	505	511	517	rBV	1404691	1647026	38.29%	6.183%
3	5.487	574	578	595	rBV	2617887	2388678	55.53%	8.967%
4	5.657	604	607	618	rBV2	160075	169164	3.93%	0.635%
5	6.098	679	682	697	rBV	228043	213621	4.97%	0.802%
6	6.481	742	747	750	rBV	2556893	2269431	52.76%	8.519%
7	6.840	805	808	816	rBV	895617	808661	18.80%	3.036%
8	6.998	831	835	853	rVB	215686	238903	5.55%	0.897%
9	7.410	900	905	908	rBV	2238474	2089399	48.57%	7.844%
10	8.122	1022	1026	1034	rBV	1323372	1041095	24.20%	3.908%
11	9.204	1205	1210	1213	rBV	4315302	3933622	91.45%	14.767%
12	9.880	1321	1325	1328	rBV	1372889	1077306	25.04%	4.044%
13	10.069	1354	1357	1370	rVB4	29749	55296	1.29%	0.208%
14	10.675	1456	1460	1470	rBV	1094362	1095150	25.46%	4.111%
15	11.375	1575	1579	1587	rBV	1032153	887890	20.64%	3.333%
16	12.633	1786	1793	1800	rBV6	18278	43412	1.01%	0.163%
17	12.974	1846	1851	1854	rBV	2974476	2739859	63.69%	10.285%
18	14.033	2027	2031	2039	rBV	761373	727611	16.92%	2.731%
19	14.463	2099	2104	2110	rVB	94655	150871	3.51%	0.566%
20	15.539	2282	2287	2297	rBV	577043	759625	17.66%	2.852%

Sum of corrected areas: 26638182

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ClientSampleId :
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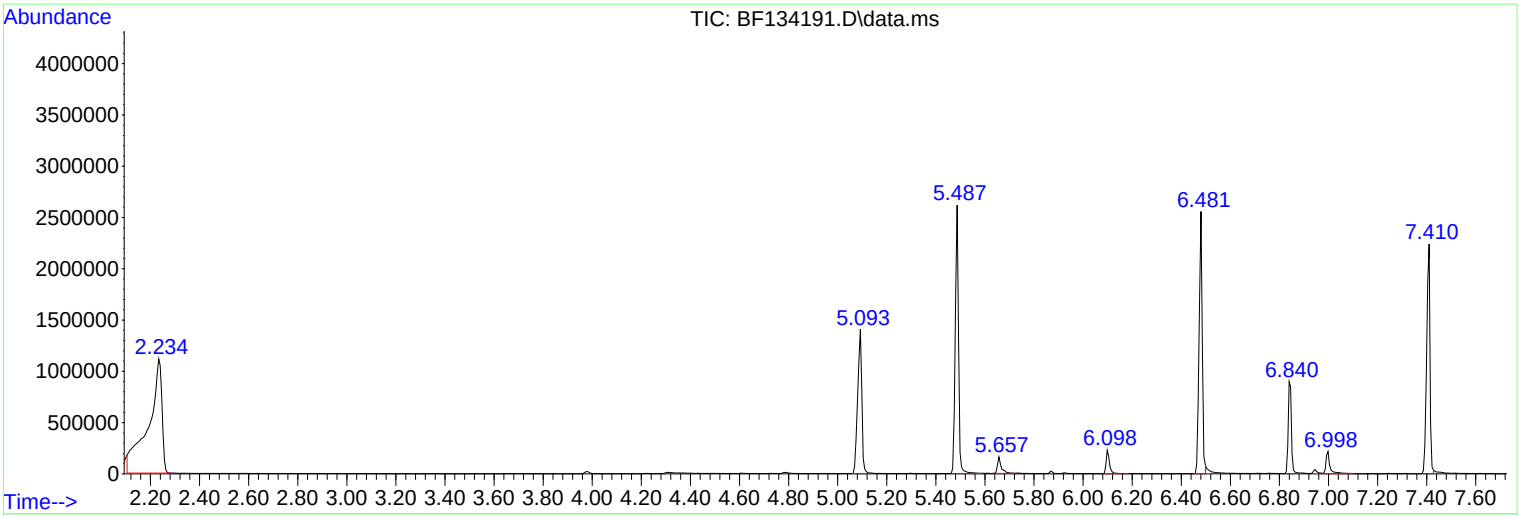
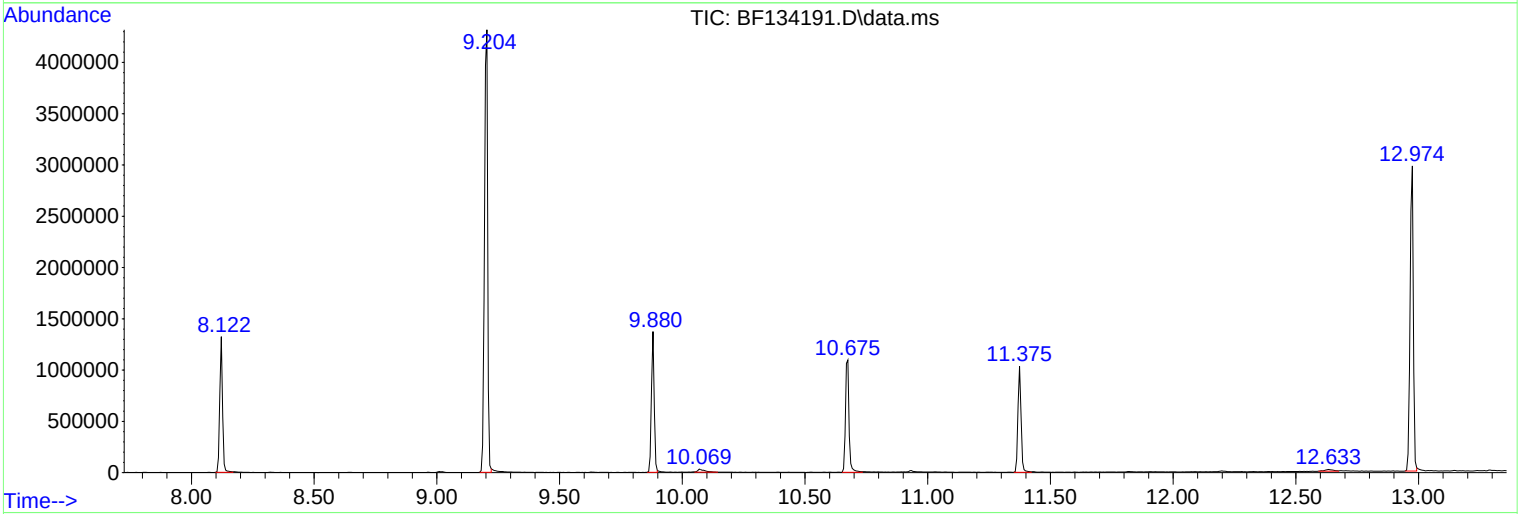
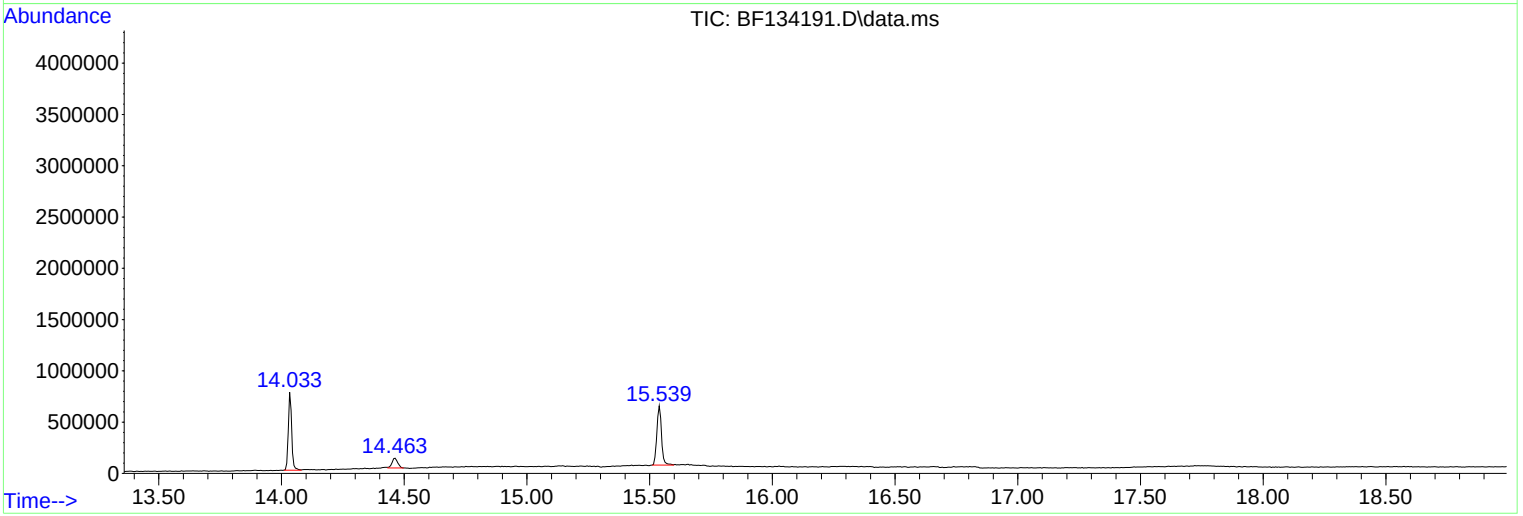
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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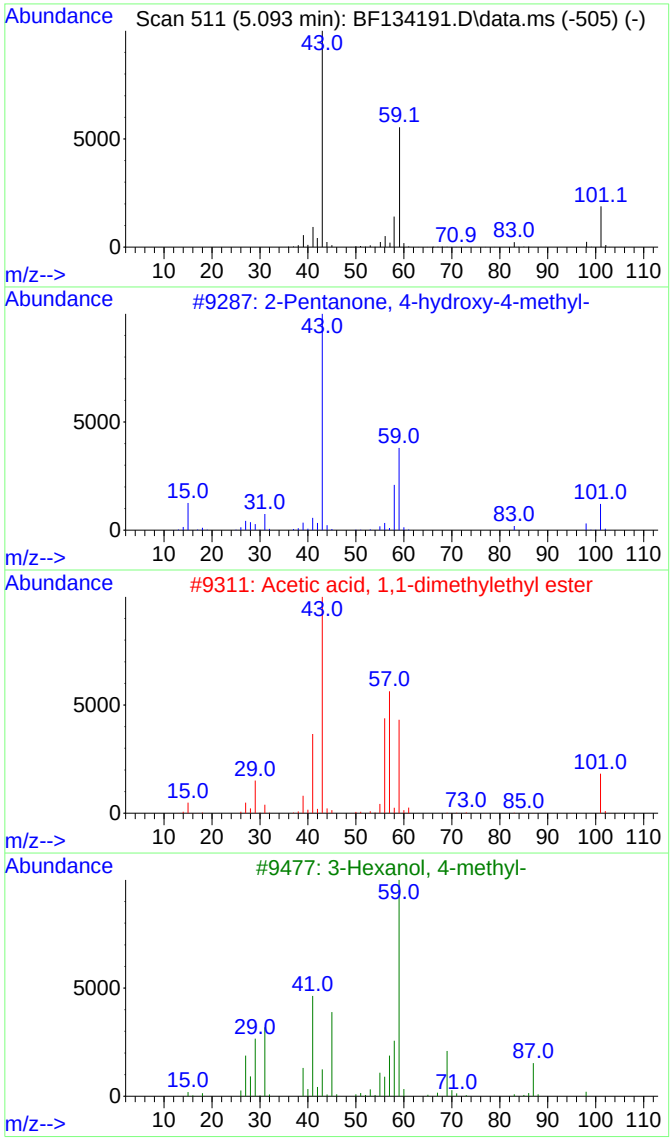
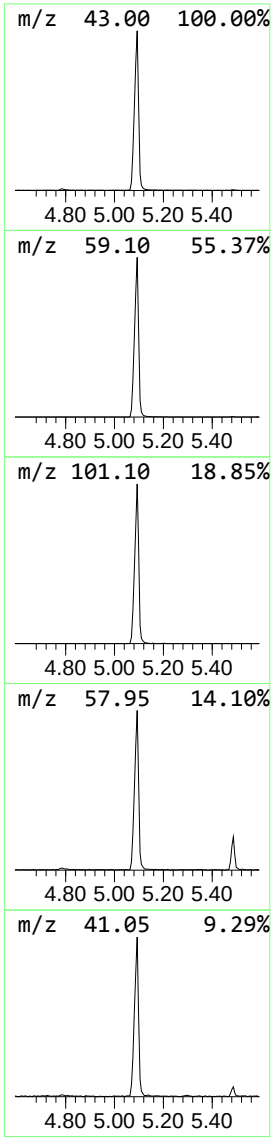
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	40.73 ng	1647030	1,4-Dichlorobenzene-d4	6.845

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





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Instrument :
BNA_F
ClientSampleId :
PB153729BL

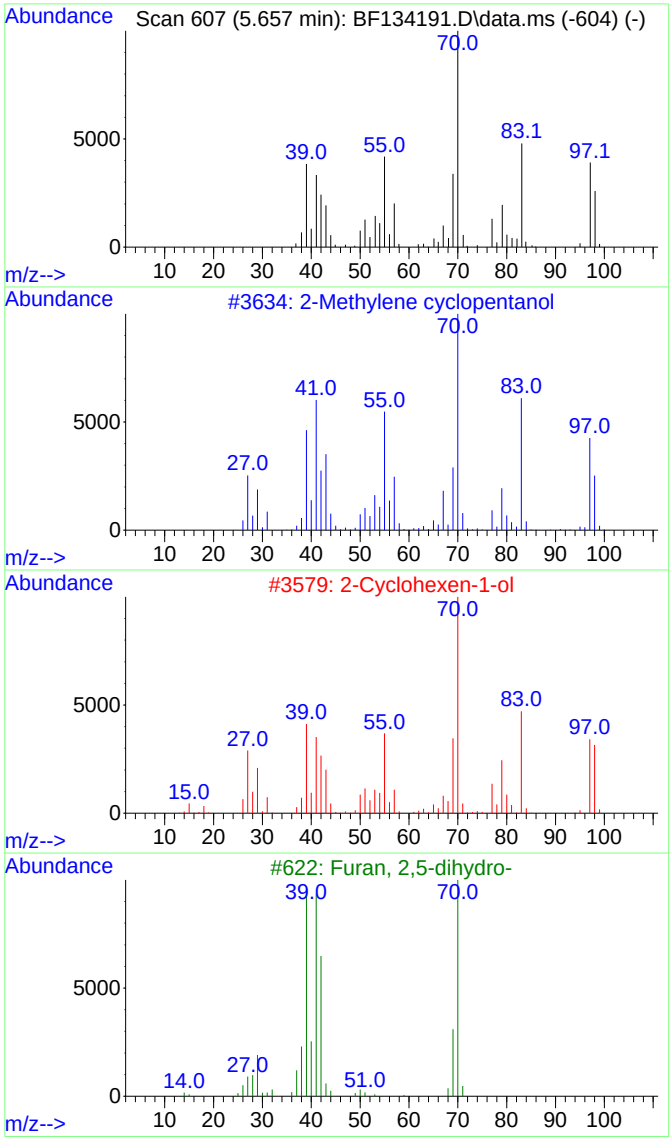
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

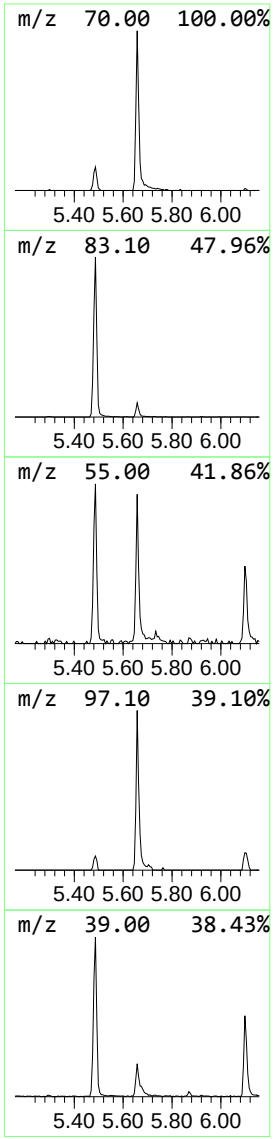
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Methylene cyclopentanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.657	4.18 ng	169164	1,4-Dichlorobenzene-d4	6.845

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methylene cyclopentanol	98	C6H10O	020461-31-8	93
2	2-Cyclohexen-1-ol	98	C6H10O	000822-67-3	93
3	Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	38
4	Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	38
5	Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	37





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Misc :
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PB153729BL

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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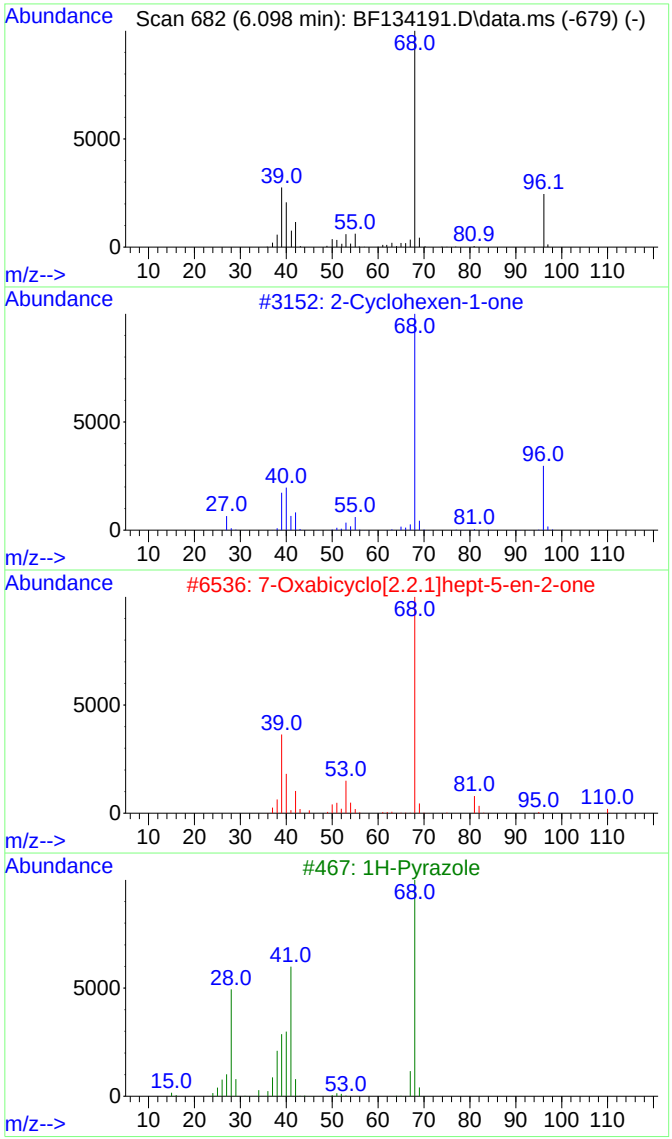
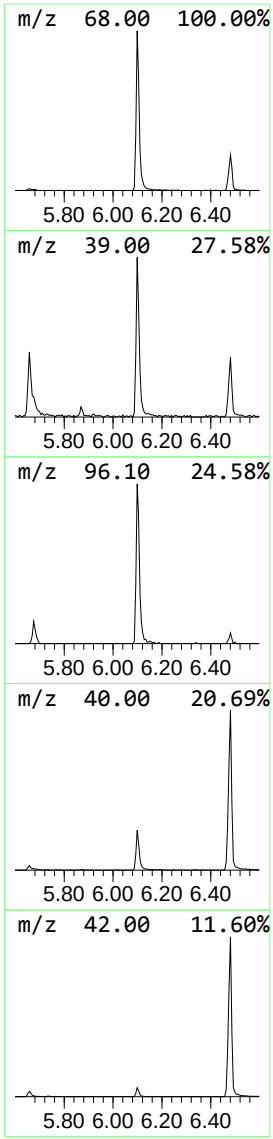
Peak Number 4 2-Cyclohexen-1-one Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.098	5.28 ng	213621	1,4-Dichlorobenzene-d4	6.845

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	91
2	7-Oxabicyclo[2.2.1]hept-5-en-2-one	110	C6H6O2	095530-78-2	53
3	1H-Pyrazole	68	C3H4N2	000288-13-1	36
4	2,5-Dihydro-3-methyl-thiophene 1...	132	C5H8O2S	001193-10-8	36
5	But-1-ene-3-yne, 1-ethoxy-	96	C6H8O	002806-41-9	14





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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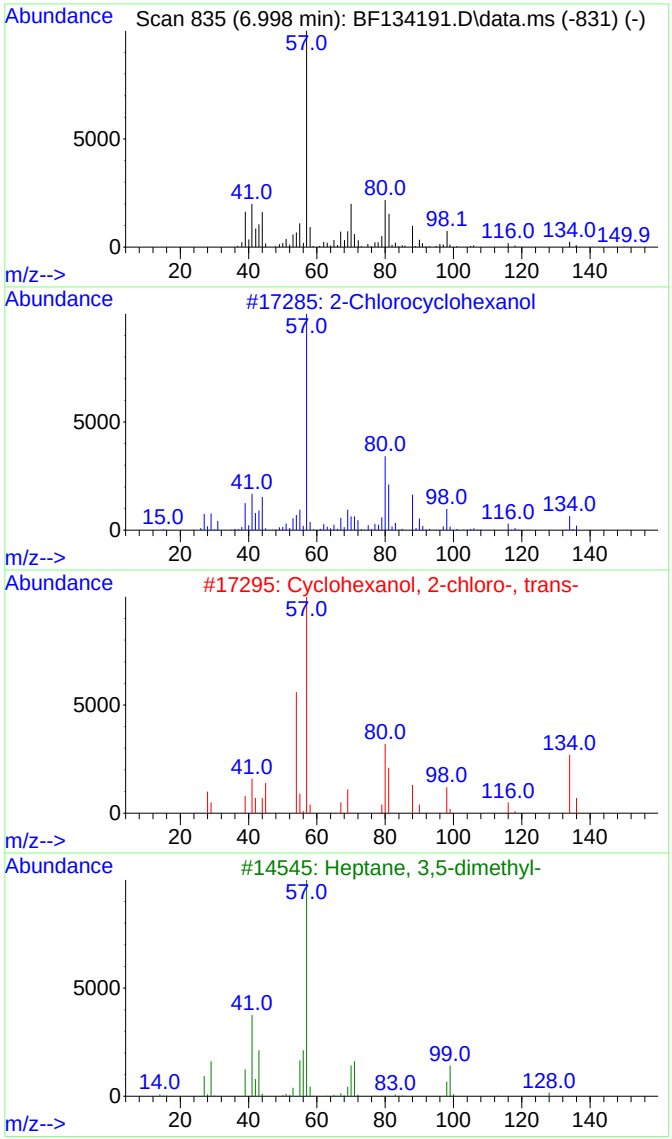
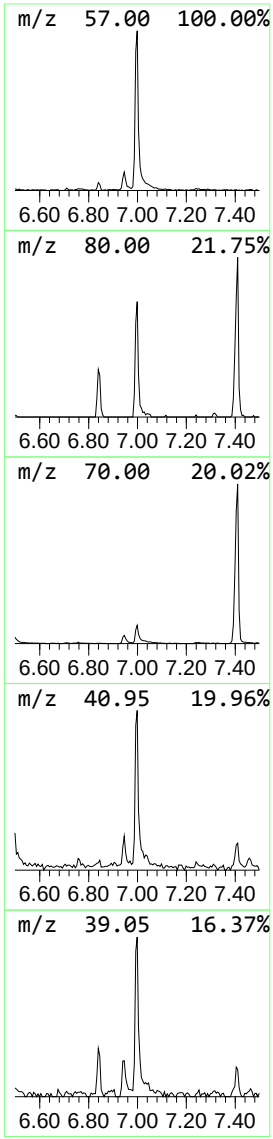
Peak Number 5 2-Chlorocyclohexanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.998	5.91 ng	238903	1,4-Dichlorobenzene-d4	6.845

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Chlorocyclohexanol	134	C6H11ClO	001561-86-0	86
2	Cyclohexanol, 2-chloro-, trans-	134	C6H11ClO	006628-80-4	37
3	Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	32
4	Cyclohexanol, 4-chloro-, trans-	134	C6H11ClO	029538-77-0	27
5	3-Furanol, tetrahydro-	88	C4H8O2	000453-20-3	25





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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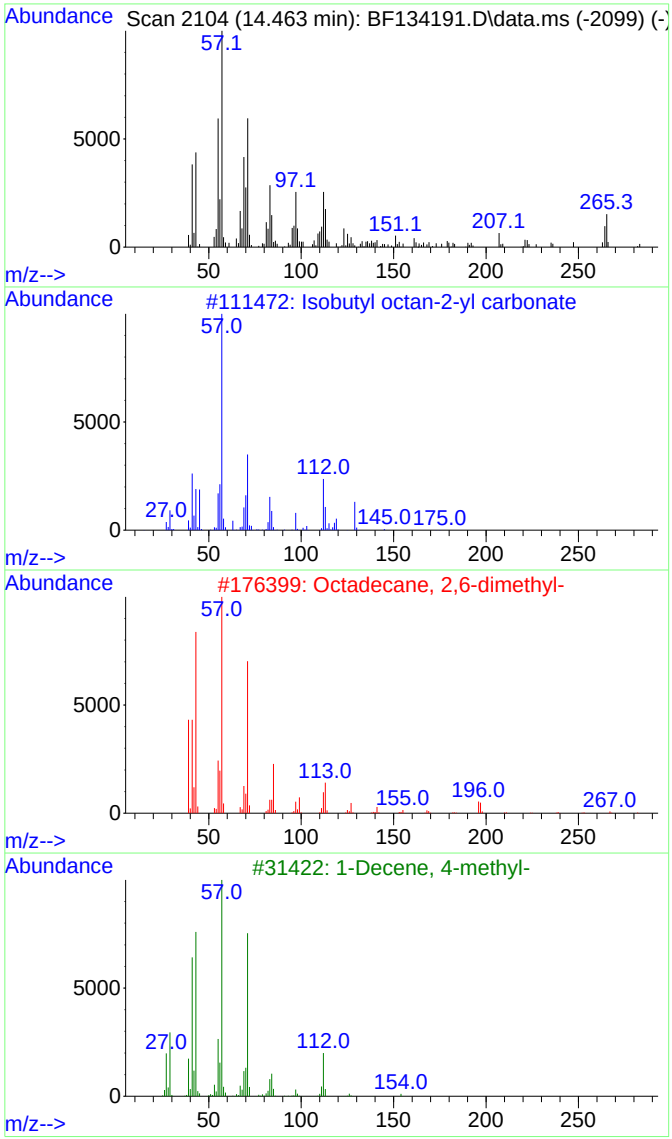
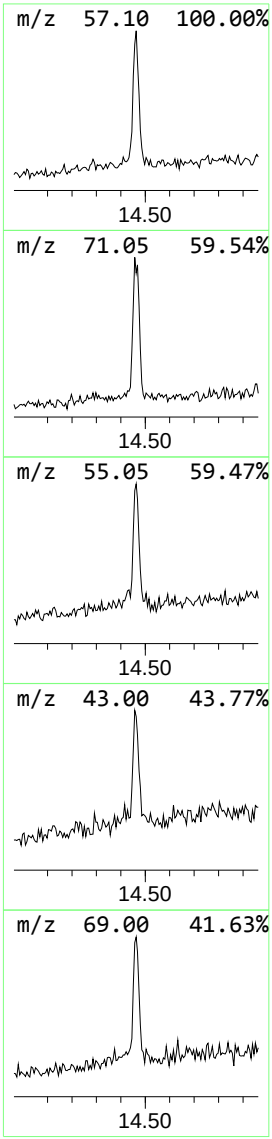
Peak Number 6 unknown14.463 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.463	4.15 ng	150871	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutyl octan-2-yl carbonate	230	C13H26O3	1000372-74-7	49
2	Octadecane, 2,6-dimethyl-	282	C20H42	075163-97-2	38
3	1-Decene, 4-methyl-	154	C11H22	013151-29-6	38
4	9-Nonadecene	266	C19H38	031035-07-1	38
5	6-Octadecenoic acid, (Z)-	282	C18H34O2	000593-39-5	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
2-Pentanone, 4-...	5.093	40.7	ng	1647030	1	6.845	808661	20.0
2-Methylene cyc...	5.657	4.2	ng	169164	1	6.845	808661	20.0
2-Cyclohexen-1-one	6.098	5.3	ng	213621	1	6.845	808661	20.0
2-Chlorocyclohe...	6.998	5.9	ng	238903	1	6.845	808661	20.0
unknown14.463	14.463	4.2	ng	150871	5	14.033	727611	20.0