LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080620\
Data File : BF121221.D
Acq On : 7 Aug 2020 00:43
Operator : JU/CG
Sample : L3576-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-0D015-03-017

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-BF071620.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.416	220	226	242	rVB	53429	96602	1.59%	0.390%
2	4.363	379	387	390	rBV	2557115	3644806	60.17%	14.701%
3	5.022	489	499	502	rBV	2807053	6057407	100.00%	24.431%
4	6.434	736	739	745	rBV2	230117	259454	4.28%	1.046%
5	6.628	768	772	777	rBV2	188695	213448	3.52%	0.861%
6	6.792	797	800	808	rBV	902534	837866	13.83%	3.379%
7	6.857	808	811	818	rVV	412590	367978	6.07%	1.484%
8	7.116	850	855	863	rVB	92021	96241	1.59%	0.388%
9	7.357	892	896	899	rBV	1618462	1511334	24.95%	6.096%
10	7.392	900	902	906	rVB	101316	83339	1.38%	0.336%
11	8.080	1016	1019	1027	rVB	991772	917722	15.15%	3.701%
12	9.157	1197	1202	1205	rBV	3160941	2947547	48.66%	11.888%
13	9.233	1213	1215	1218	rVV	105408	88363	1.46%	0.356%
14	9.551	1265	1269	1276	rBV	219302	232335	3.84%	0.937%
15	9.833	1313	1317	1328	rBV	1140839	1035994	17.10%	4.178%
16	10.216	1377	1382	1384	rBV	64558	67348	1.11%	0.272%
17	10.986	1510	1513	1517	rVV3	52764	64950	1.07%	0.262%
18	11.021	1517	1519	1524	rVV	51954	61798	1.02%	0.249%
19	11.186	1541	1547	1550	rBV	67501	65551	1.08%	0.264%
20	11.321	1566	1570	1582	rBV	1039207	1070956	17.68%	4.319%
21	12.021	1686	1689	1693	rBV	79034	68381	1.13%	0.276%
22	12.292	1732	1735	1739	rBV	82290	86873	1.43%	0.350%
23	12.410	1752	1755	1759	rVB	68524	63863	1.05%	0.258%
24	12.910	1835	1840	1843	rBV	2801372	2662739	43.96%	10.740%
25	13.810	1990	1993	2004	rBV	256531	414374	6.84%	1.671%
26	13.962	2016	2019	2025	rVB	887176	860390	14.20%	3.470%
27	14.427	2096	2098	2101	rVB2	86229	69929	1.15%	0.282%
28	15.421	2262	2267	2273	rBV	602622	846093	13.97%	3.413%

Sum of corrected areas: 24793681

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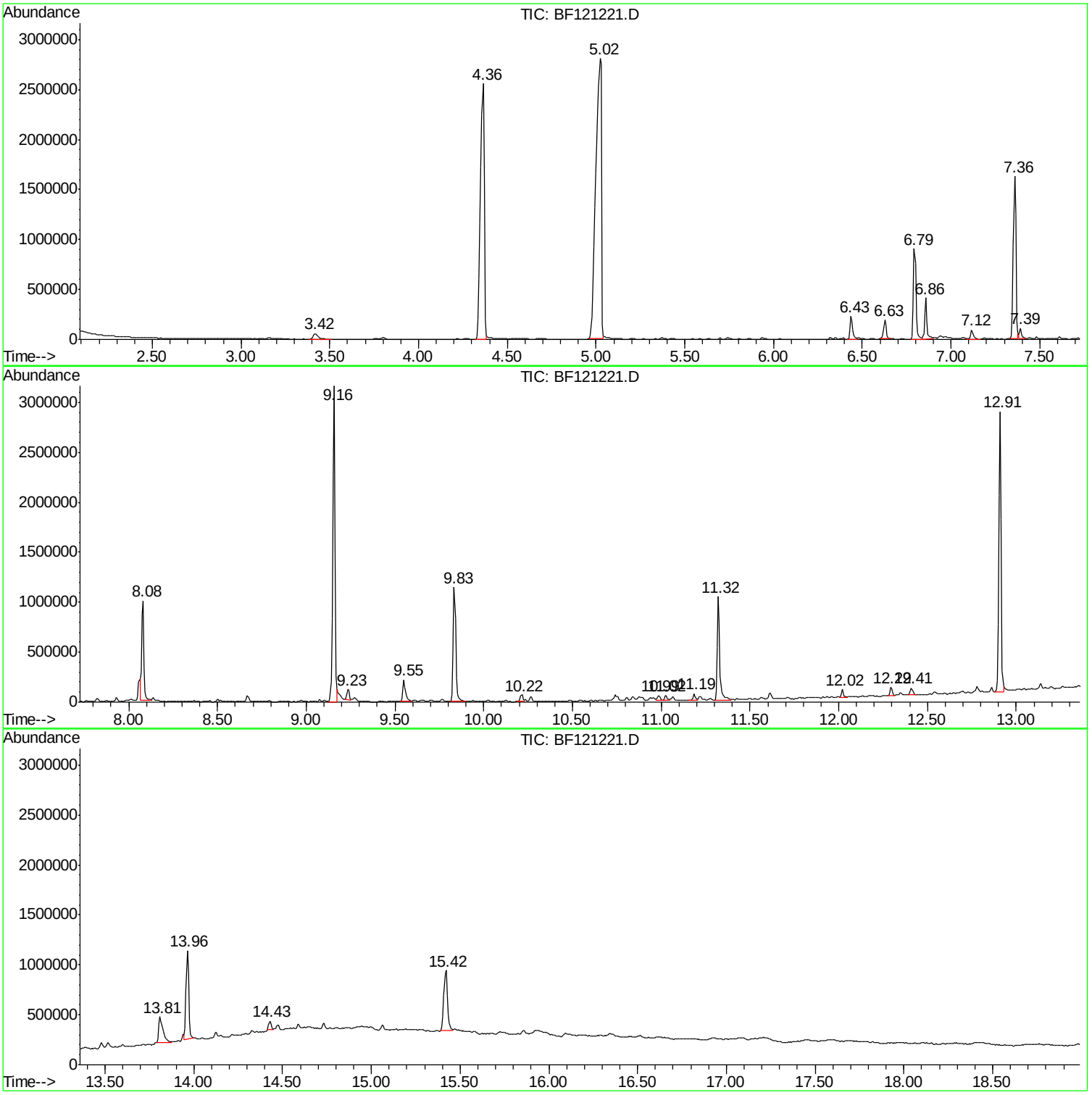
Instrument :
BNA_F
ClientSampleId :
FK-0D015-03-017

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

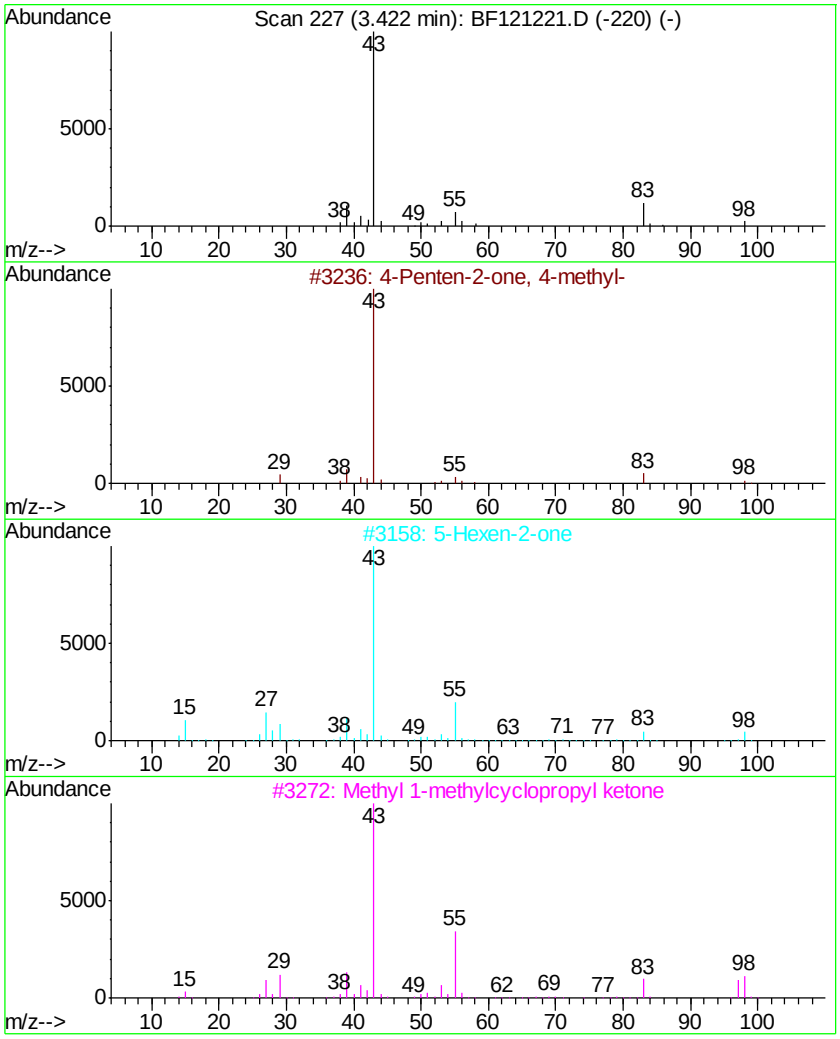
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

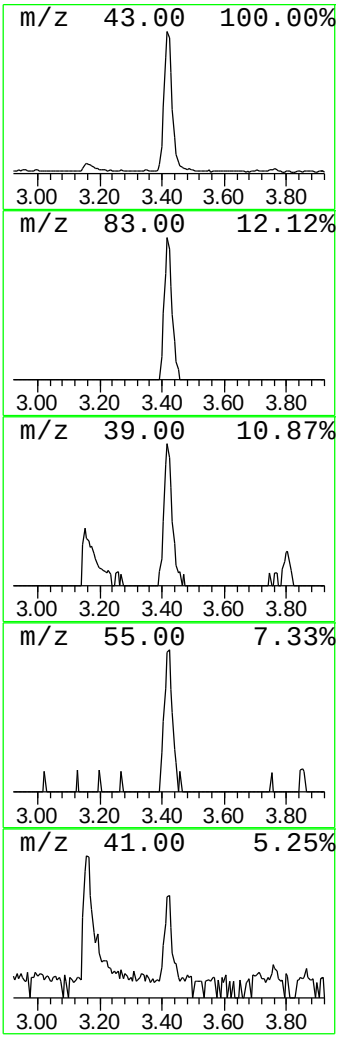
****

Peak Number 1 4-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.42	2.31 ng	96602	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	80
2	5-Hexen-2-one	98	C6H10O	000109-49-9	53
3	Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	47
4	2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	17
5	Isoxazole, 5-methyl-	83	C4H5NO	005765-44-6	9





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Operator : JU/CG
Sample : L3576-01
Misc :
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Instrument : BNA_F
ClientSampleId : FK-0D015-03-017

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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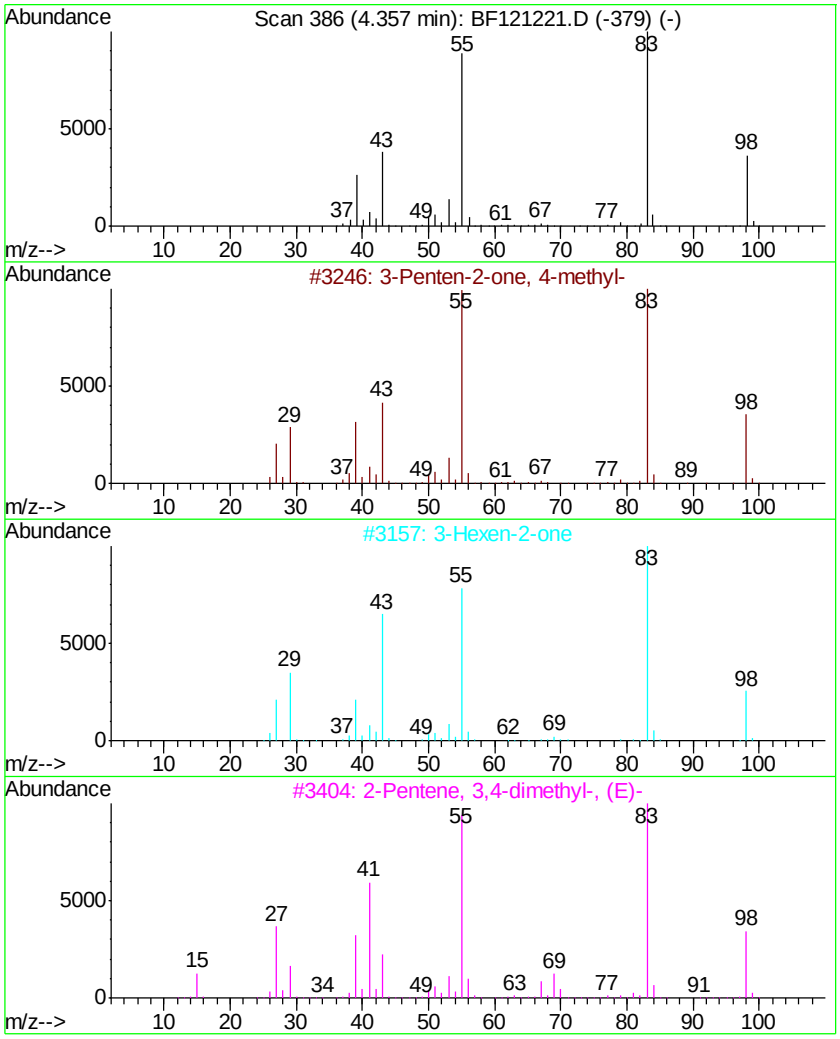
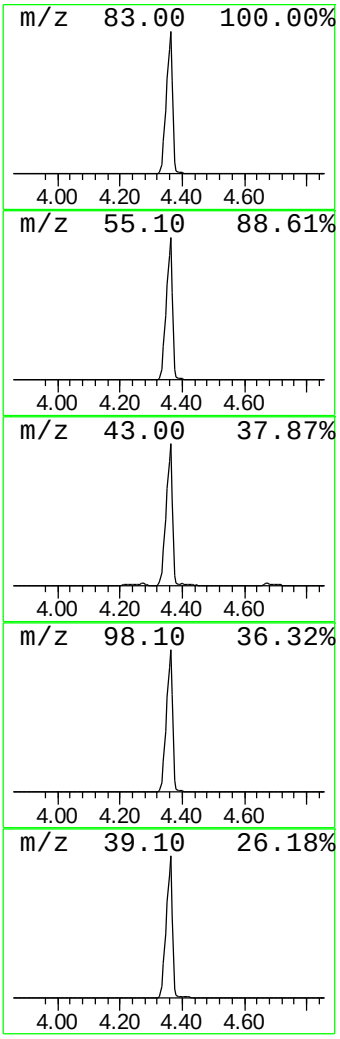
Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.36	87.00 ng	3644810	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080620\
Data File : BF121221.D
Acq On : 7 Aug 2020 00:43
Operator : JU/CG
Sample : L3576-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-0D015-03-017

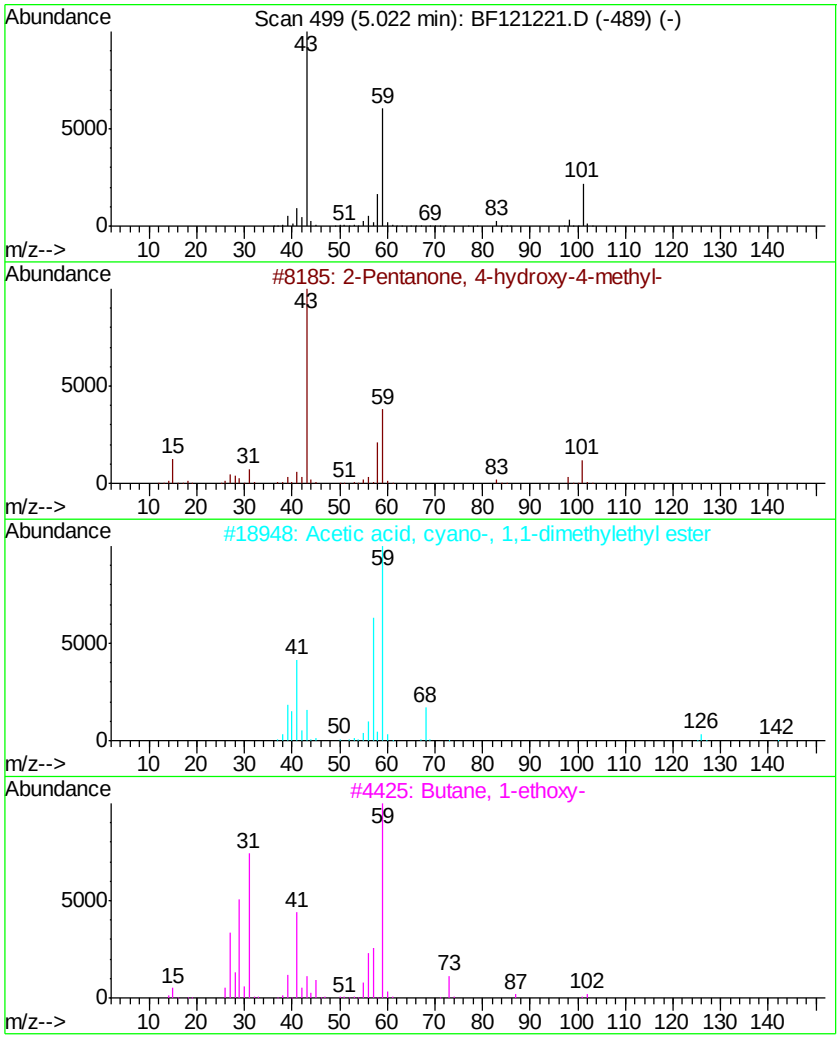
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

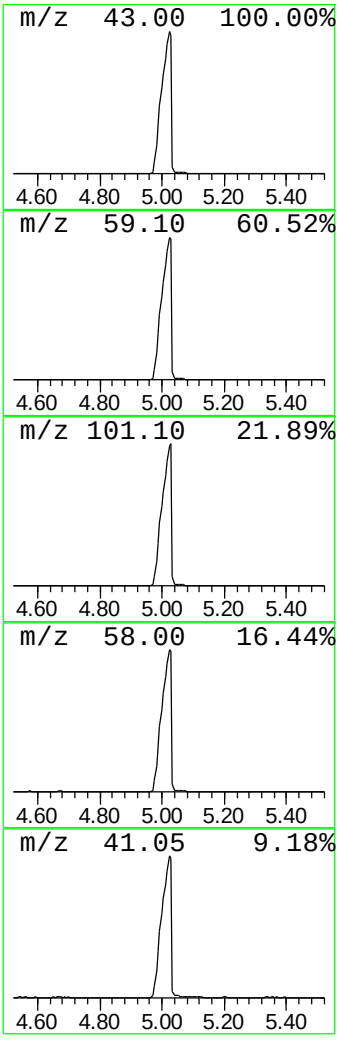
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	144.59 ng	6057410	1,4-Dichlorobenzene-d4	6.79

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





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Acq On : 7 Aug 2020 00:43
Operator : JU/CG
Sample : L3576-01
Misc :
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Instrument : BNA_F
ClientSampleId : FK-0D015-03-017

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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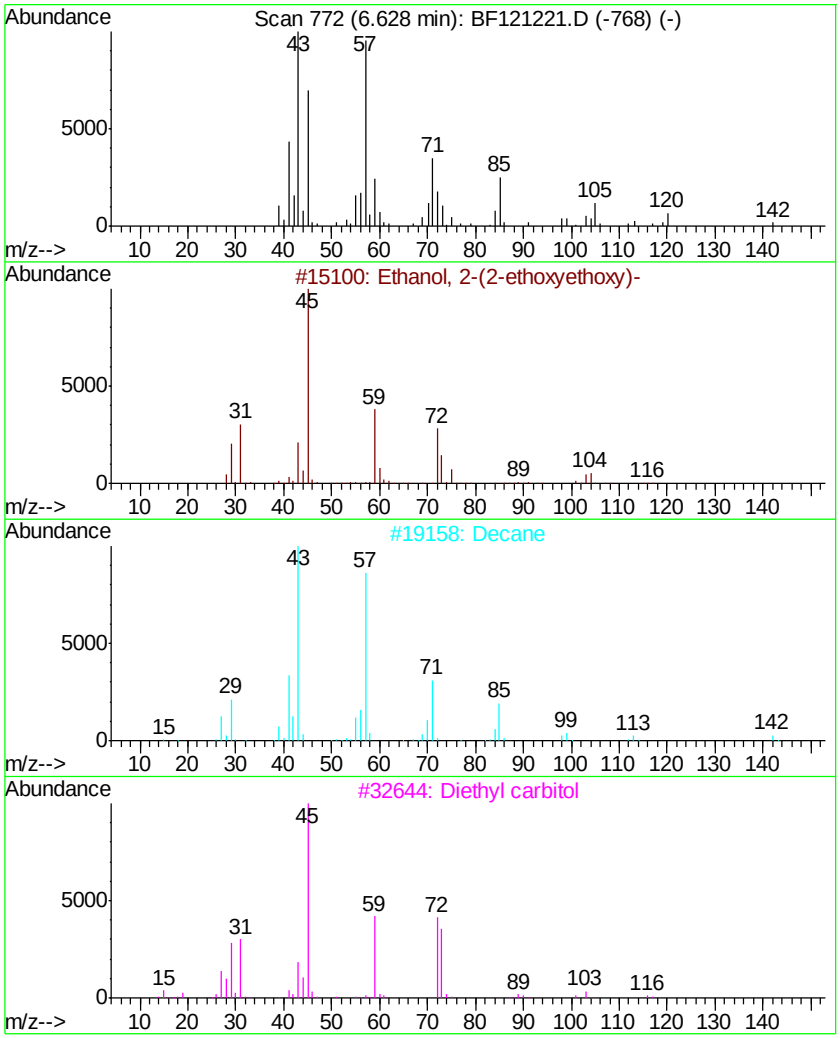
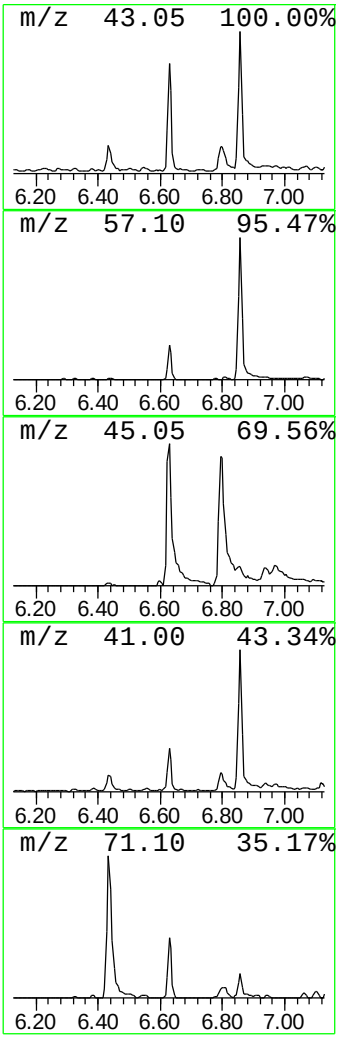
Peak Number 4 unknown6.63 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	5.10 ng	213448	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	43
2	Decane	142	C10H22	000124-18-5	42
3	Diethyl carbitol	162	C8H18O3	000112-36-7	38
4	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	27
5	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	27





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Operator : JU/CG
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Misc :
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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

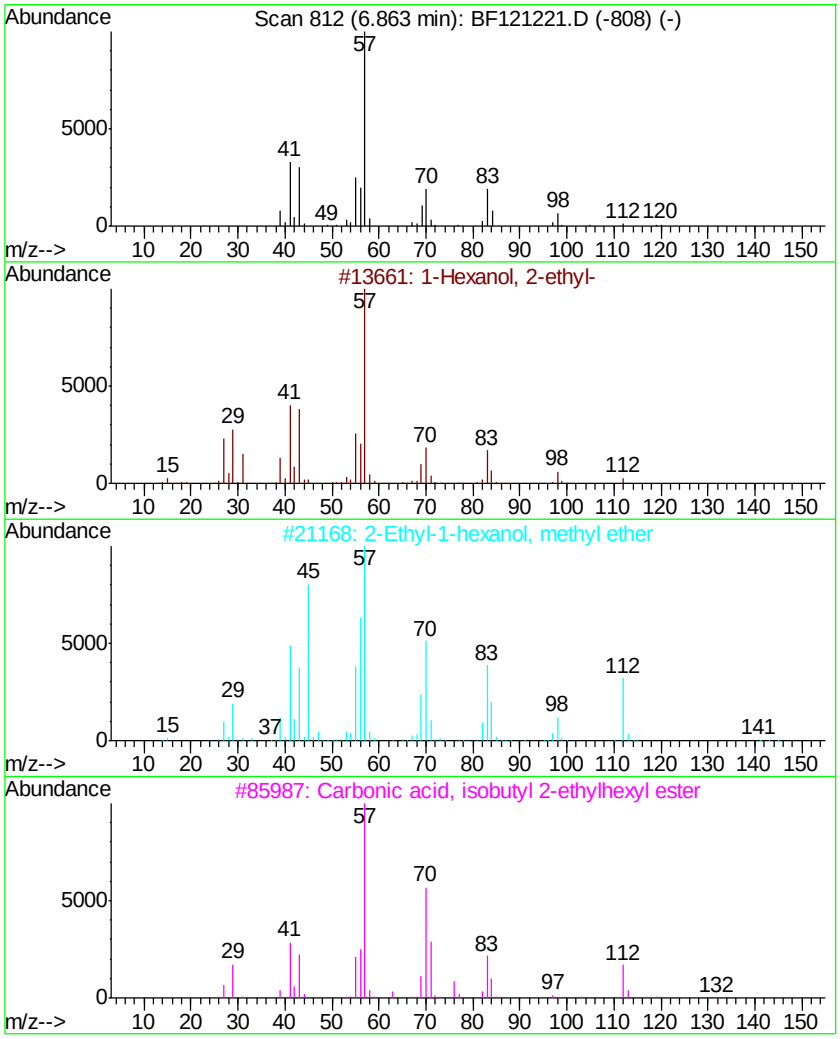
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

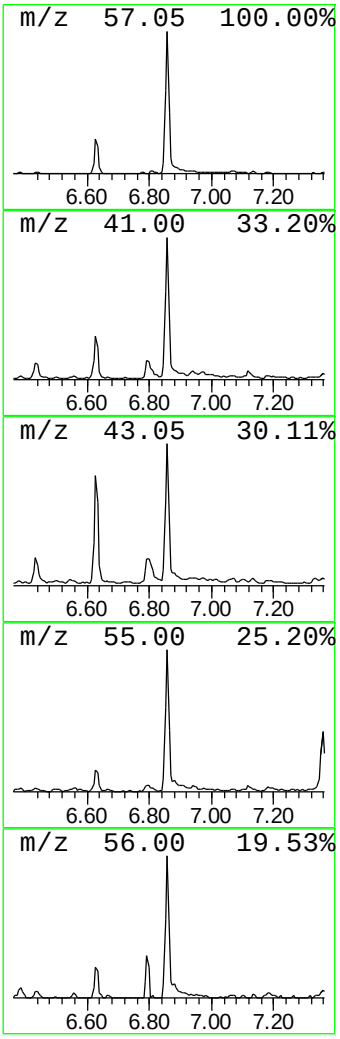
****

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.86	8.78 ng	367978	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
2	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	50
3	Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000357-82-9	50
4	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
5	Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	45





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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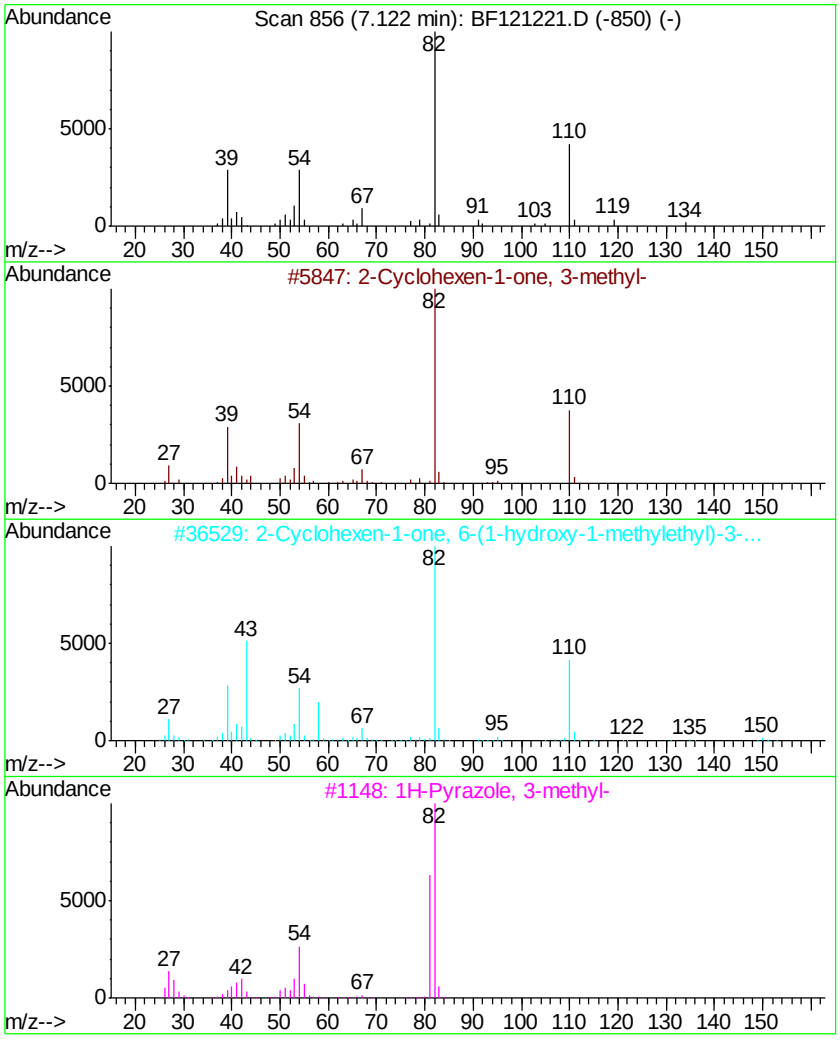
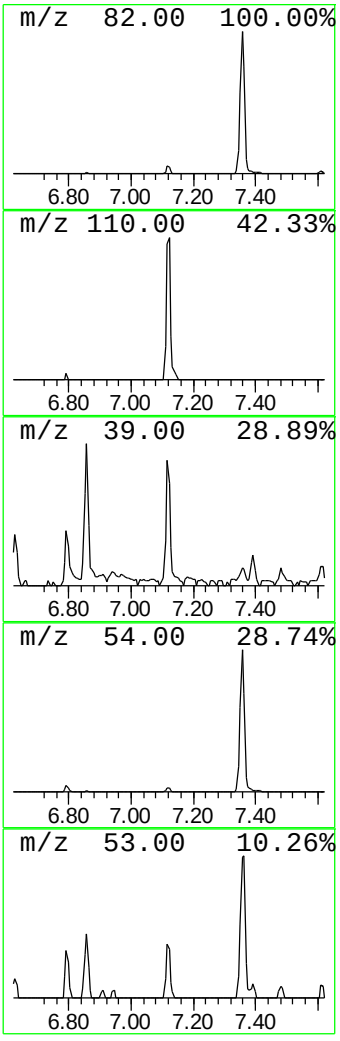
Peak Number 6 2-Cyclohexen-1-one, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.12	2.30 ng	96241	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-one, 3-methyl-	110	C7H10O	001193-18-6	87
2	2-Cyclohexen-1-one, 6-(1-hydroxy...	168	C10H16O2	087791-00-2	56
3	1H-Pyrazole, 3-methyl-	82	C4H6N2	001453-58-3	53
4	2-Cyclohexen-1-one, 3,5-dimethyl-	124	C8H12O	001123-09-7	50
5	2-Cyclopenten-1-one	82	C5H6O	000930-30-3	50





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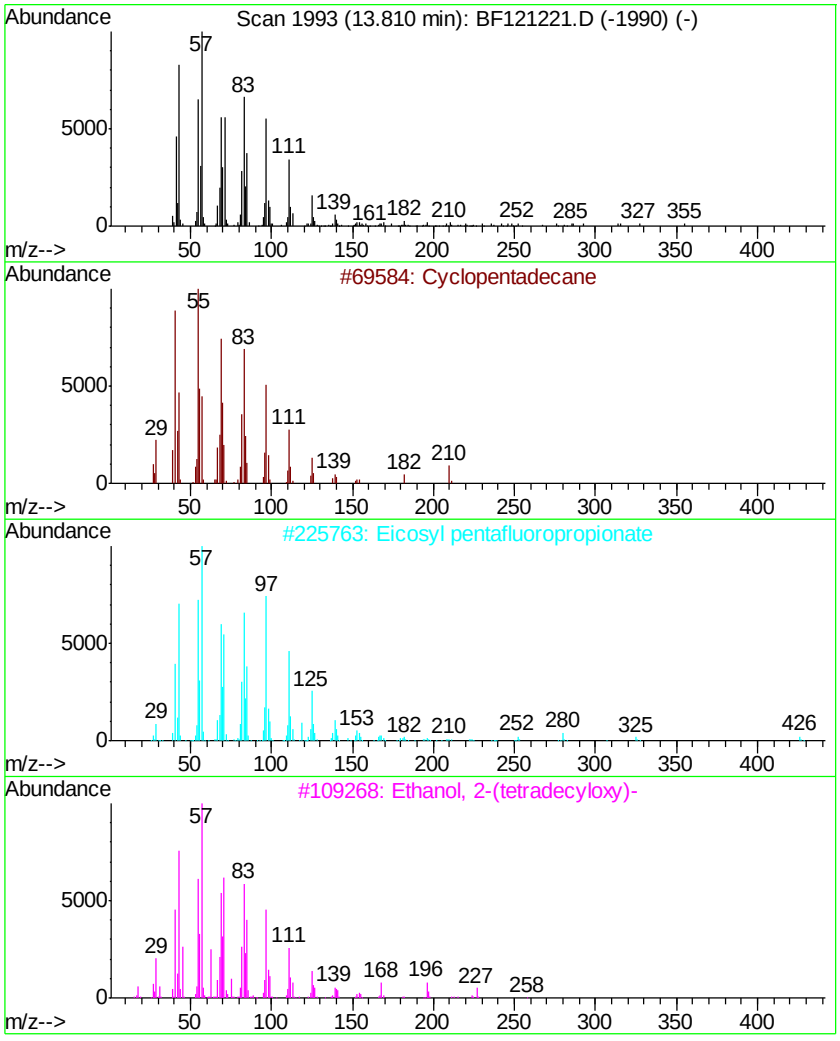
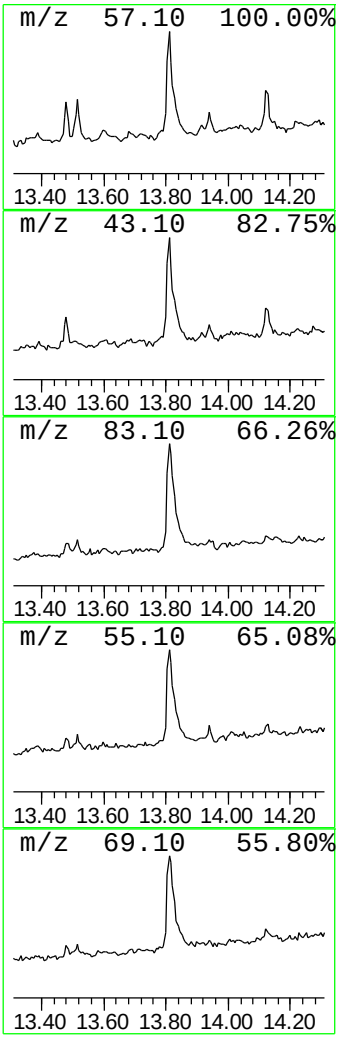
Peak Number 7 Cyclopentadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	9.63 ng	414374	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	95
2	Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	91
3	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
4	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
5	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91





Tentatively Identified Compound (LSC) summary

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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
4-Penten-2-one, 4...	3.42	2.3	ng	96602	1	6.79	837866	20.0
3-Penten-2-one, 4...	4.36	87.0	ng	3644810	1	6.79	837866	20.0
2-Pentanone, 4-hy...	5.02	144.6	ng	6057410	1	6.79	837866	20.0
unknown6.63	6.63	5.1	ng	213448	1	6.79	837866	20.0
1-Hexanol, 2-ethyl-	6.86	8.8	ng	367978	1	6.79	837866	20.0
2-Cyclohexen-1-on...	7.12	2.3	ng	96241	1	6.79	837866	20.0
Cyclopentadecane	13.81	9.6	ng	414374	5	13.96	860390	20.0