LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100217\
Data File : BF099020.D
Acq On : 3 Oct 2017 00:42
Operator : SJ/JU
Sample : I5531-01 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G-62-0-2.5

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:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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	2.175	13	15	34	rVB	55305	123482	14.26%	1.383%
2	4.504	408	411	418	rBV	121054	137220	15.84%	1.537%
3	5.116	511	515	530	rBV	579997	539365	62.28%	6.041%
4	5.516	579	583	593	rVB	271029	234477	27.07%	2.626%
5	6.522	750	754	764	rBV	557583	478747	55.28%	5.362%
6	6.669	775	779	783	rBV	465898	356378	41.15%	3.992%
7	6.904	815	819	822	rBV	882900	703585	81.24%	7.880%
8	7.057	841	845	849	rBV	565791	462369	53.39%	5.179%
9	7.463	910	914	917	rBV	358664	309120	35.69%	3.462%
10	8.186	1033	1037	1040	rBV	1092385	866091	100.00%	9.700%
11	9.257	1215	1219	1229	rBV	708887	585838	67.64%	6.561%
12	9.333	1229	1232	1237	rVB3	11394	11174	1.29%	0.125%
13	9.651	1283	1286	1293	rBV	87514	71340	8.24%	0.799%
14	9.863	1318	1322	1327	rBV	17452	16249	1.88%	0.182%
15	9.945	1332	1336	1339	rBV	924076	798169	92.16%	8.940%
16	10.363	1400	1407	1410	rBV2	27253	28208	3.26%	0.316%
17	10.586	1441	1445	1447	rBV2	9784	10766	1.24%	0.121%
18	10.833	1485	1487	1497	rVB2	30911	44797	5.17%	0.502%
19	11.280	1561	1563	1566	rBV	25342	22329	2.58%	0.250%
20	11.310	1566	1568	1574	rVB3	16492	18808	2.17%	0.211%
21	11.433	1585	1589	1592	rBV	794859	701725	81.02%	7.859%
22	11.457	1592	1593	1595	rVB	25314	12076	1.39%	0.135%
23	11.710	1633	1636	1639	rBV	28858	23821	2.75%	0.267%
24	12.116	1703	1705	1708	rBV	30201	23590	2.72%	0.264%
25	12.504	1769	1771	1775	rVB	41479	32559	3.76%	0.365%
26	12.645	1792	1795	1798	rBV	43550	37296	4.31%	0.418%
27	12.874	1828	1834	1836	rBV	102869	135241	15.62%	1.515%
28	13.010	1851	1857	1863	rBV	562780	483139	55.78%	5.411%
29	13.233	1892	1895	1898	rBV	50993	40655	4.69%	0.455%
30	13.486	1935	1938	1942	rVB	66000	52335	6.04%	0.586%
31	13.574	1951	1953	1958	rBV	48894	42955	4.96%	0.481%
32	13.904	2006	2009	2011	rBV	55334	47909	5.53%	0.537%
33	14.074	2034	2038	2041	rBV	750858	716985	82.78%	8.030%
34	14.221	2060	2063	2065	rBV	52442	49271	5.69%	0.552%

LSC Area Percent Report

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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:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.521	2112	2114	2117	rVB2	58859	49213	5.68%	0.551%
36	15.568	2287	2292	2299	rVB	511191	661136	76.34%	7.405%

Sum of corrected areas: 8928418

LSC Report - Integrated Chromatogram

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Data File : BF099020.D
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Operator : SJ/JU
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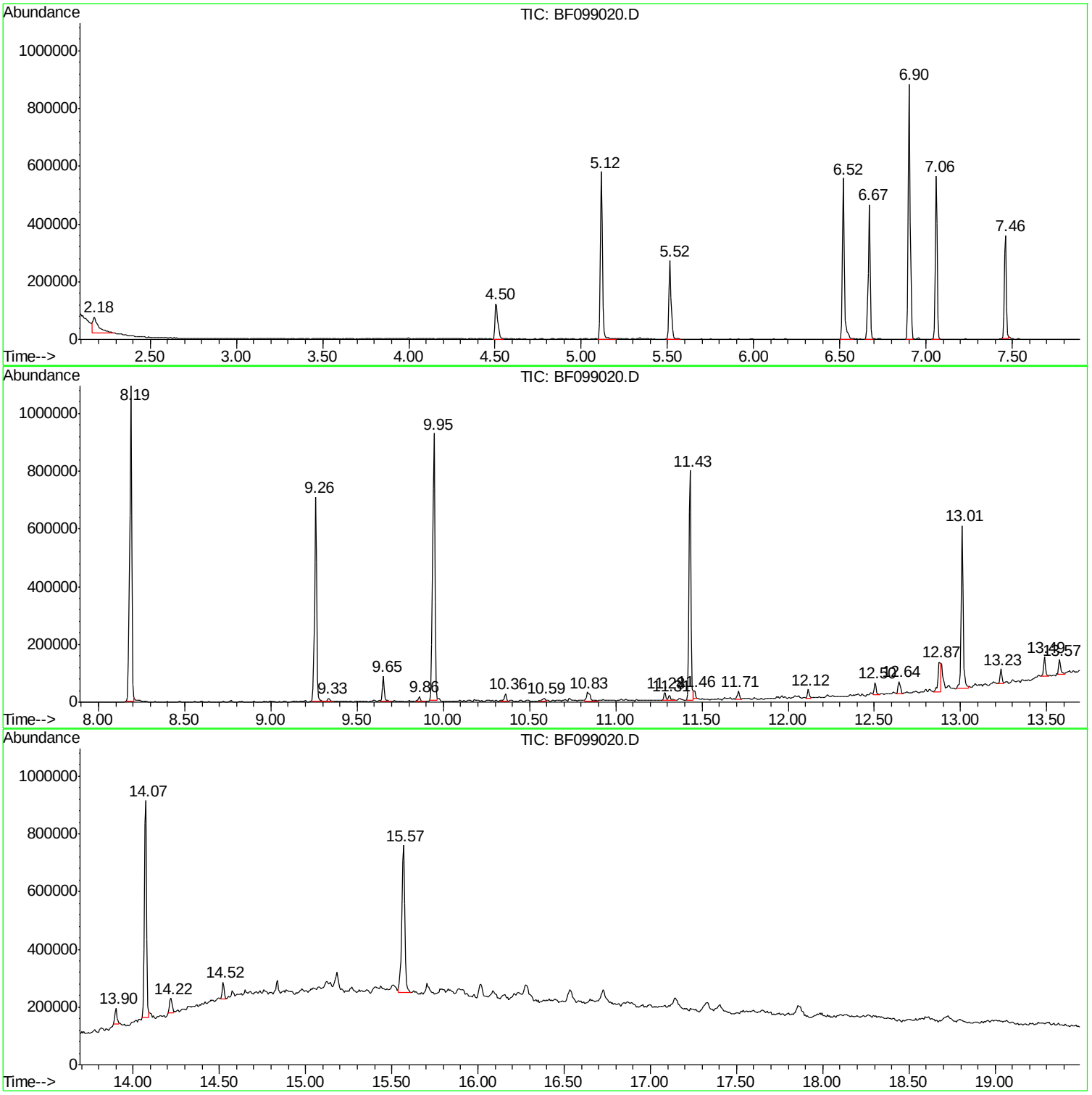
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G-62-0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100217\
Data File : BF099020.D
Acq On : 3 Oct 2017 00:42
Operator : SJ/JU
Sample : I5531-01 5X
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Instrument : BNA_F
ClientSampleId : G-62-0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

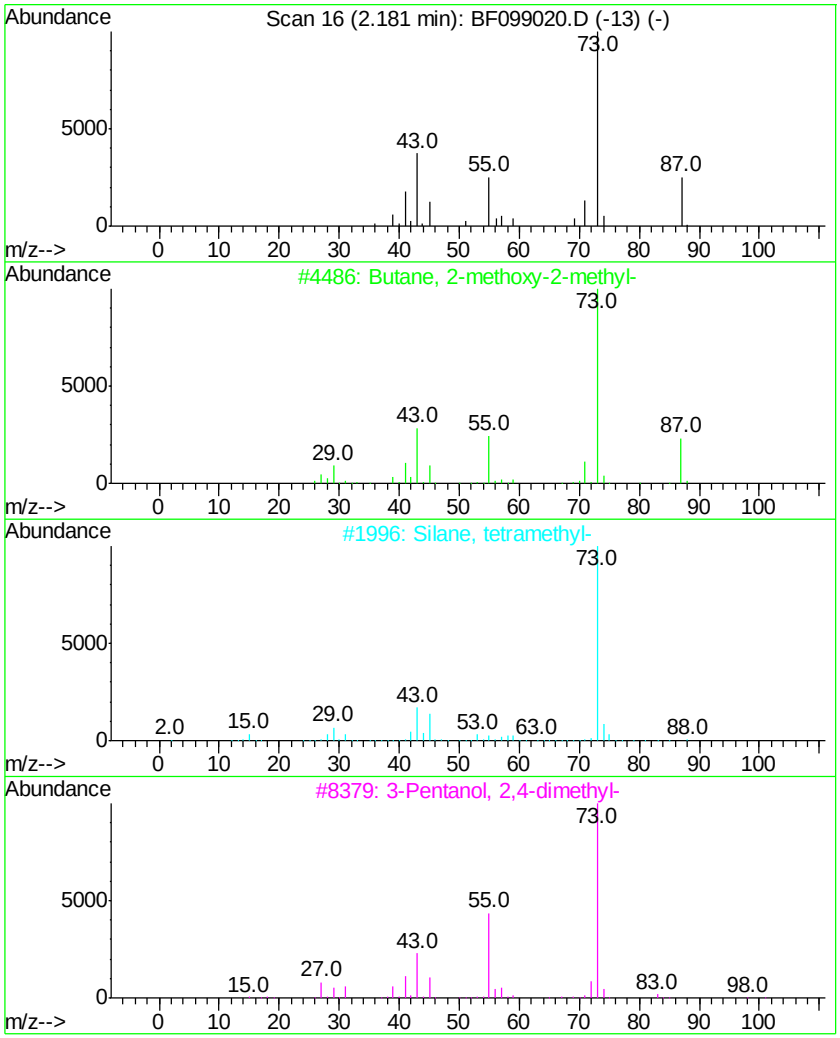
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

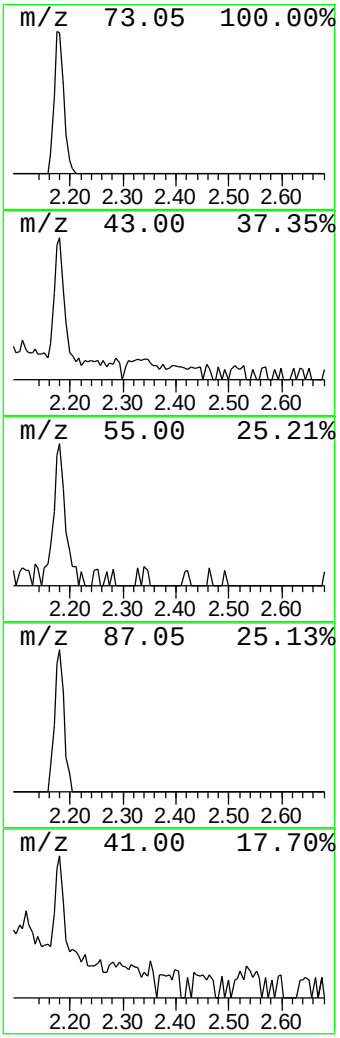
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.18	3.51 ng	123482	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9
4	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9
5	1-Propene-1-thiol	74	C3H6S	000925-89-3	7





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Acq On : 3 Oct 2017 00:42
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Sample : I5531-01 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G-62-0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

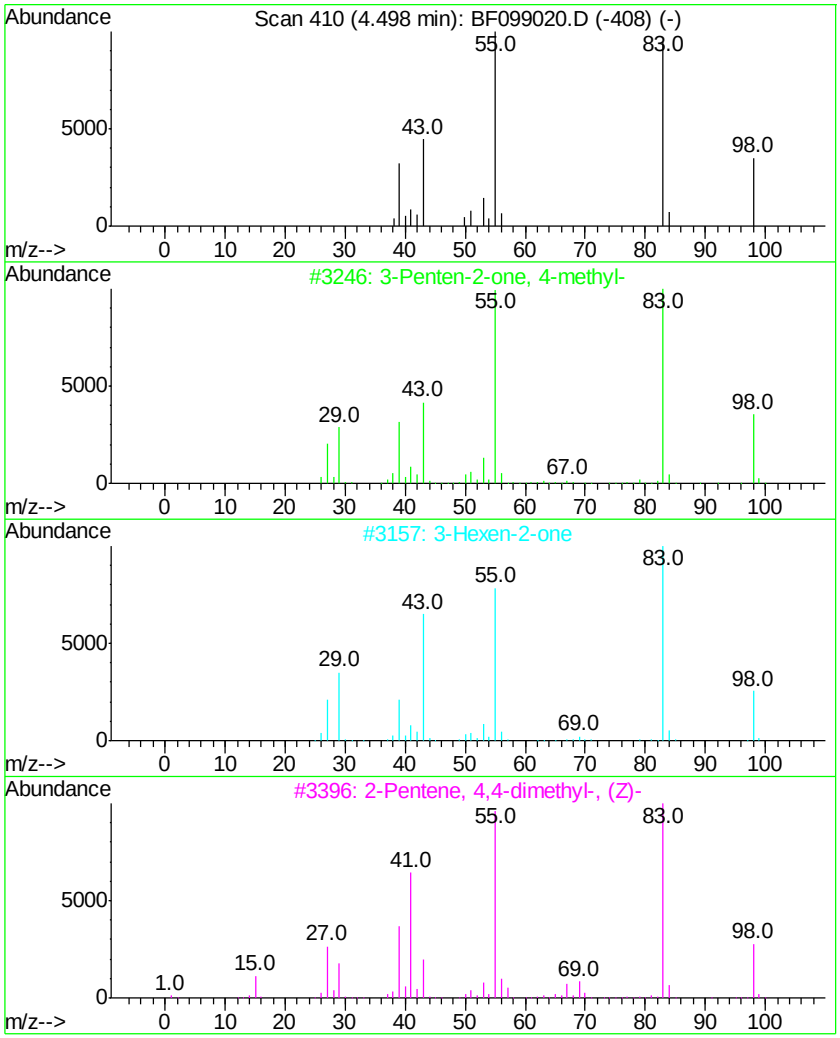
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

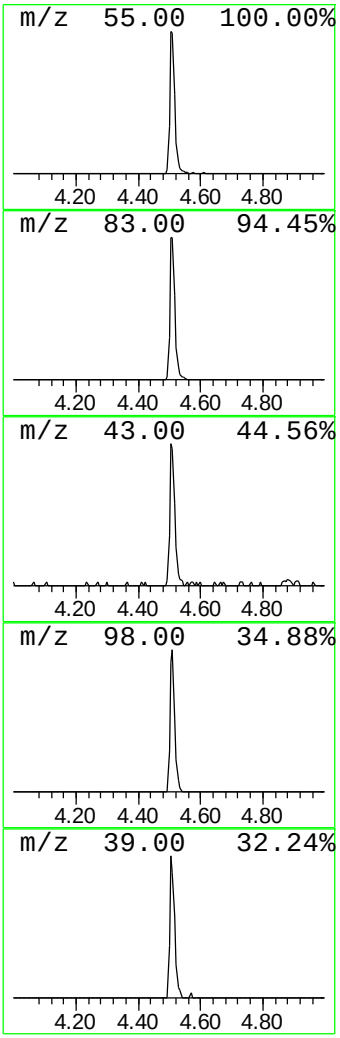
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.50	3.90 ng	137220	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86
4	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100217\
Data File : BF099020.D
Acq On : 3 Oct 2017 00:42
Operator : SJ/JU
Sample : I5531-01 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G-62-0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

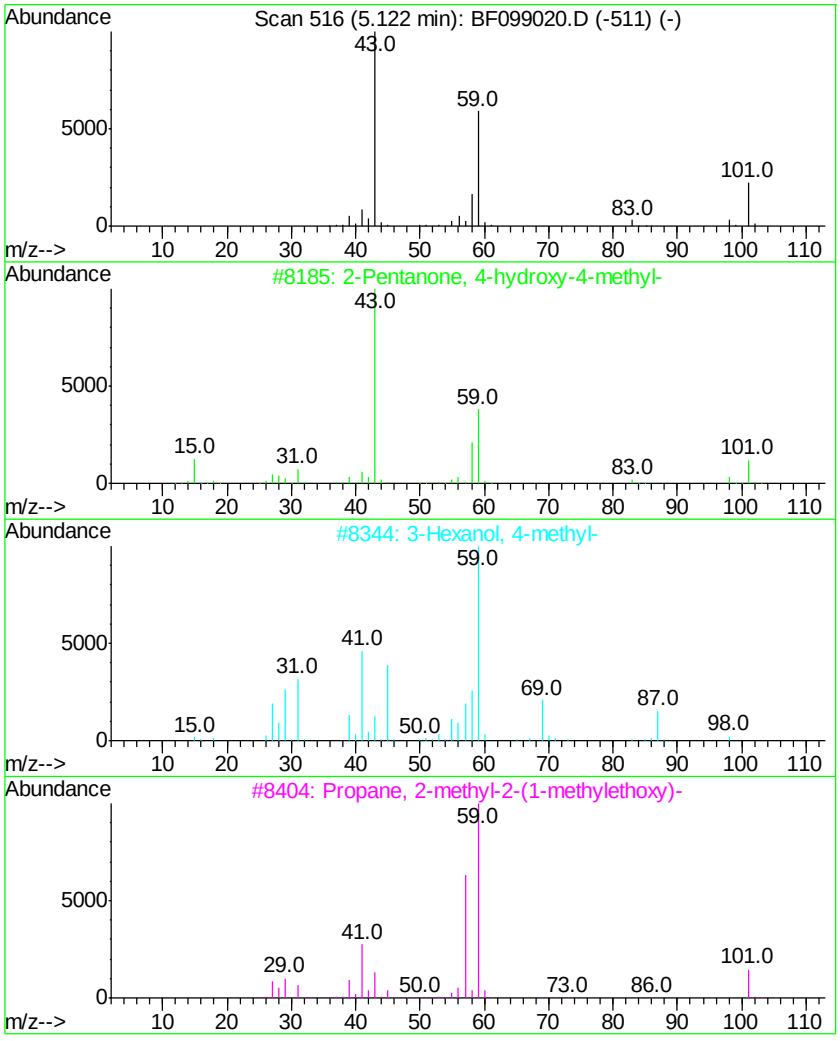
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

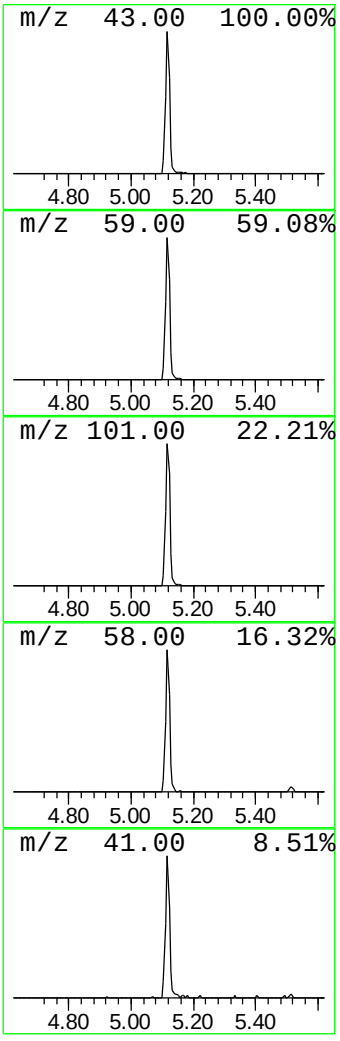
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	15.33 ng	539365	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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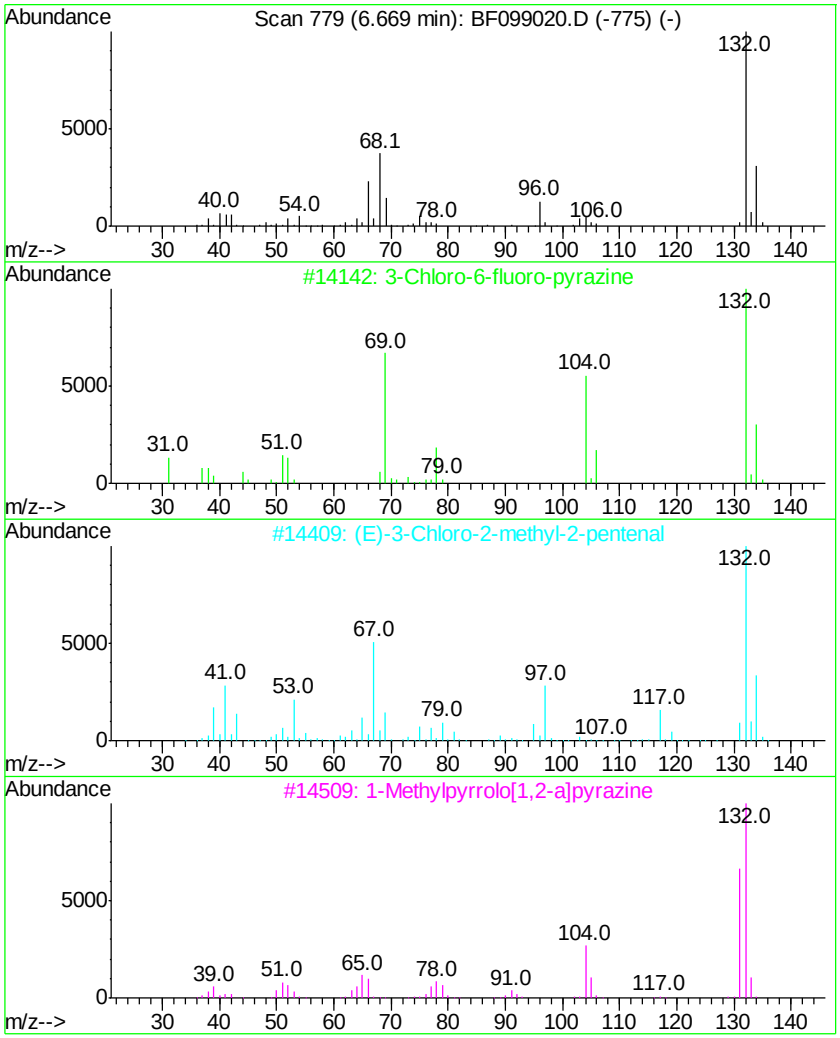
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

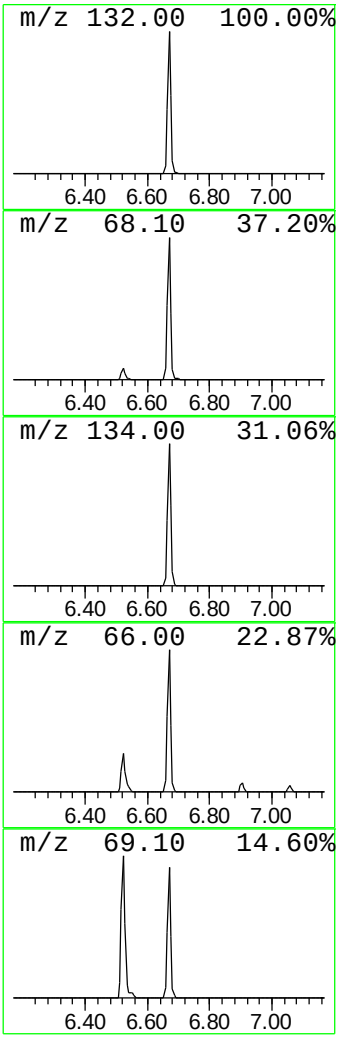
****

Peak Number 4 unknown6.67 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	10.13 ng	356378	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.18	3.5	ng	123482	1	6.90	703585	20.0
3-Penten-2-one, 4...	4.50	3.9	ng	137220	1	6.90	703585	20.0
2-Pentanone, 4-hy...	5.12	15.3	ng	539365	1	6.90	703585	20.0
unknown6.67	6.67	10.1	ng	356378	1	6.90	703585	20.0