LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080921\
Data File : BF125020.D
Acq On : 10 Aug 2021 1:23
Operator : JU/CG
Sample : M3291-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-1

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-BF080421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125020.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	11	13	16	rBB	1391	1261	1.15%	0.139%
2	5.040	496	502	505	rBV	63408	75477	68.79%	8.347%
3	5.446	567	571	574	rBV	129933	109725	100.00%	12.135%
4	5.834	635	637	640	rBB	15521	11935	10.88%	1.320%
5	6.463	740	744	746	rBV	112465	108388	98.78%	11.987%
6	6.822	802	805	808	rBB	35681	27215	24.80%	3.010%
7	7.387	897	901	904	rBB	80389	69622	63.45%	7.700%
8	8.004	1003	1006	1009	rBV	34264	23933	21.81%	2.647%
9	8.104	1019	1023	1026	rBB	40515	33145	30.21%	3.666%
10	9.175	1202	1205	1208	rBV	124993	99338	90.53%	10.986%
11	9.857	1318	1321	1324	rBB	44554	32266	29.41%	3.568%
12	10.645	1452	1455	1458	rBB	73310	54477	49.65%	6.025%
13	11.339	1570	1573	1576	rBV	33852	27613	25.17%	3.054%
14	11.863	1660	1662	1664	rBB	2817	1706	1.55%	0.189%
15	12.433	1755	1759	1761	rBB	1634	1347	1.23%	0.149%
16	12.551	1777	1779	1782	rBB	5306	4114	3.75%	0.455%
17	12.780	1816	1818	1821	rBB	4519	3702	3.37%	0.409%
18	12.927	1839	1843	1846	rBB	111729	88899	81.02%	9.832%
19	13.433	1926	1929	1932	rBV3	1194	1665	1.52%	0.184%
20	13.810	1991	1993	1999	rBV2	4944	6192	5.64%	0.685%
21	13.892	2003	2007	2008	rBV	1391	1487	1.36%	0.164%
22	13.980	2016	2022	2025	rBV	36601	30292	27.61%	3.350%
23	14.139	2048	2049	2052	rVB2	2219	1500	1.37%	0.166%
24	14.174	2052	2055	2056	rBV	1741	1813	1.65%	0.201%
25	14.186	2056	2057	2060	rBV	1231	1375	1.25%	0.152%
26	14.321	2078	2080	2084	rBV2	1735	2743	2.50%	0.303%
27	14.451	2097	2102	2103	rBV2	2430	2912	2.65%	0.322%
28	14.510	2109	2112	2114	rVB4	1353	1409	1.28%	0.156%
29	14.539	2114	2117	2121	rBV4	2112	3406	3.10%	0.377%
30	14.733	2148	2150	2152	rVB3	2016	1935	1.76%	0.214%
31	14.757	2152	2154	2160	rVV4	1880	2264	2.06%	0.250%
32	14.815	2160	2164	2167	rVV4	3394	4115	3.75%	0.455%
33	14.863	2170	2172	2174	rVV2	1563	1401	1.28%	0.155%
34	14.880	2174	2175	2178	rVB3	1789	1323	1.21%	0.146%
35	14.951	2184	2187	2188	rBV2	2028	1483	1.35%	0.164%
36	14.968	2188	2190	2194	rVB4	1641	2096	1.91%	0.232%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080921\
Data File : BF125020.D
Acq On : 10 Aug 2021 1:23
Operator : JU/CG
Sample : M3291-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-1

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-BF080421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.004	2194	2196	2201	rBV5	3557	5663	5.16%	0.626%
38	15.151	2219	2221	2223	rBV3	1704	1522	1.39%	0.168%
39	15.274	2237	2242	2244	rBV5	1277	1376	1.25%	0.152%
40	15.374	2257	2259	2261	rVB2	2686	1979	1.80%	0.219%
41	15.439	2265	2270	2276	rVB	20388	25167	22.94%	2.783%
42	15.545	2286	2288	2289	rBV2	1816	1289	1.17%	0.143%
43	15.733	2318	2320	2322	rBV3	1265	1242	1.13%	0.137%
44	15.815	2331	2334	2338	rBV3	1622	2458	2.24%	0.272%
45	15.845	2338	2339	2343	rBV4	1341	1475	1.34%	0.163%
46	15.921	2348	2352	2353	rBV	2002	2182	1.99%	0.241%
47	15.992	2361	2364	2367	rVB4	1890	2728	2.49%	0.302%
48	16.362	2426	2427	2429	rBV2	1823	1312	1.20%	0.145%
49	16.545	2456	2458	2461	rVB	1703	1882	1.72%	0.208%
50	16.745	2488	2492	2493	rBV3	1247	1278	1.16%	0.141%
51	16.880	2514	2515	2518	rBV3	1301	1260	1.15%	0.139%
52	16.921	2520	2522	2524	rVB3	1559	1583	1.44%	0.175%
53	17.368	2595	2598	2601	rBV3	1116	1495	1.36%	0.165%
54	17.439	2608	2610	2614	rVB2	1328	1698	1.55%	0.188%
55	18.004	2704	2706	2709	rVB2	1542	1454	1.33%	0.161%
56	18.598	2804	2807	2810	rVB2	1230	1586	1.45%	0.175%

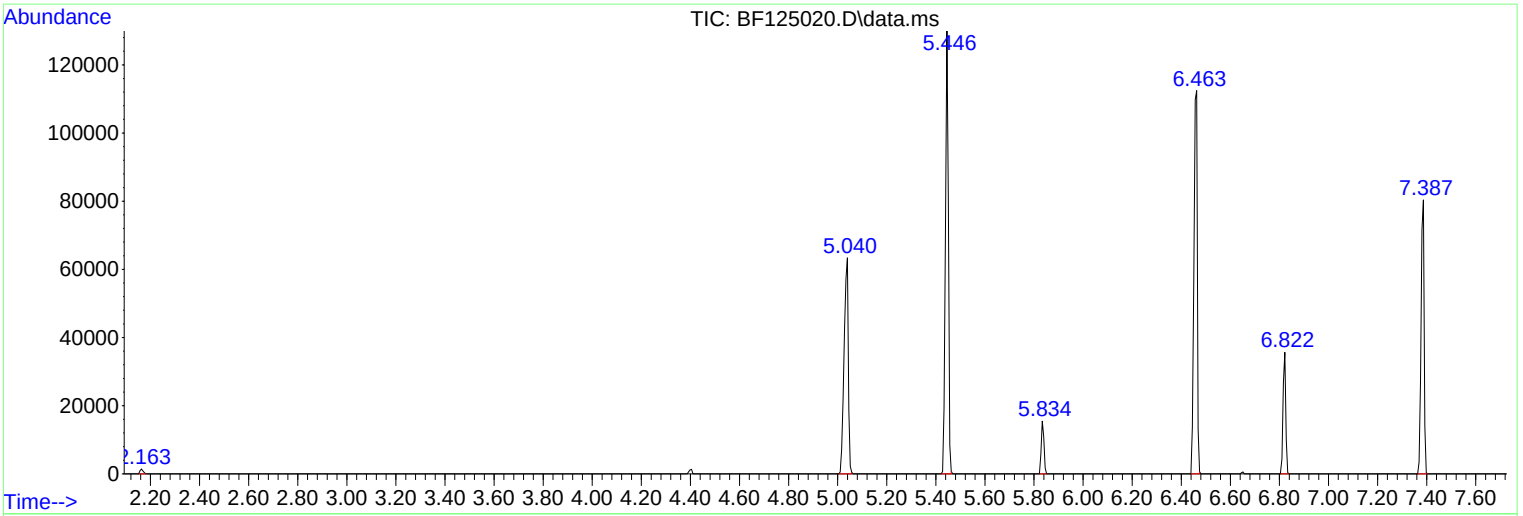
Sum of corrected areas: 904203

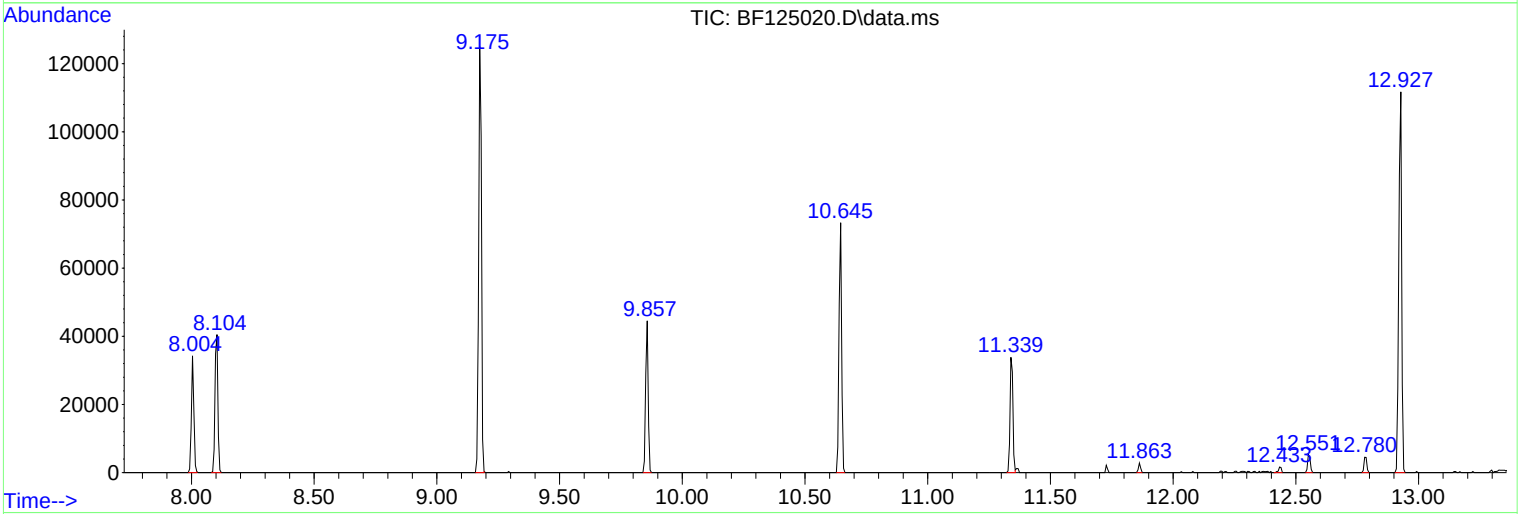
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080921\
Data File : BF125020.D
Acq On : 10 Aug 2021 1:23
Operator : JU/CG
Sample : M3291-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

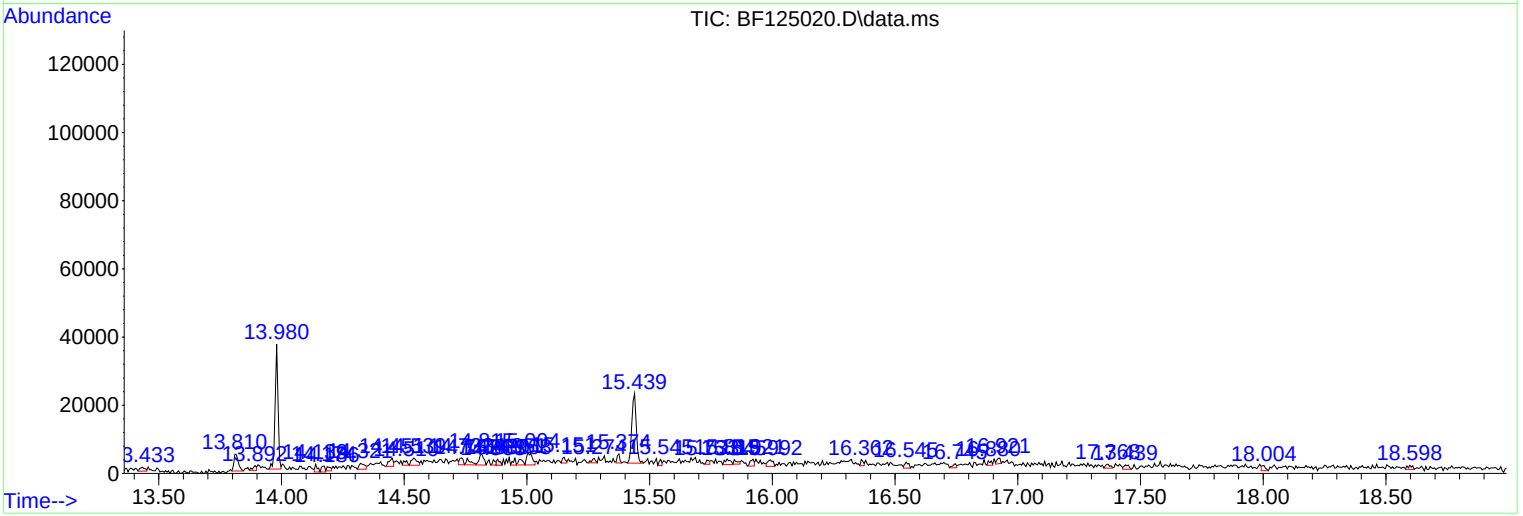
Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.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_F\Data\BF080921\
Data File : BF125020.D
Acq On : 10 Aug 2021 1:23
Operator : JU/CG
Sample : M3291-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
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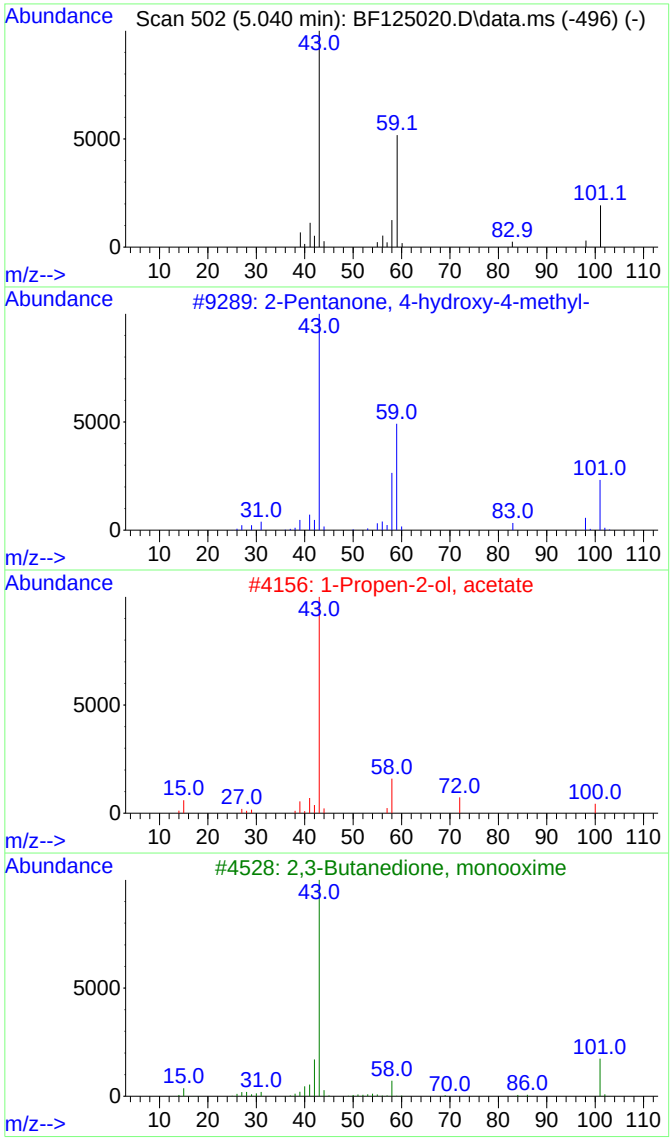
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

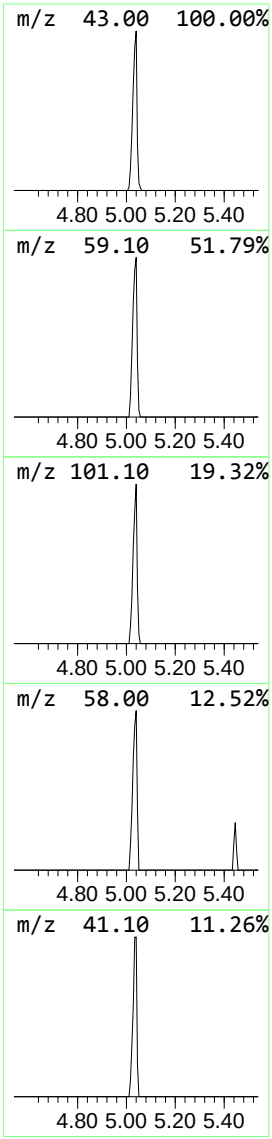
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.040	55.47 ng	75477	1,4-Dichlorobenzene-d4	6.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	3-Octanol	130	C8H18O	000589-98-0	9
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080921\
Data File : BF125020.D
Acq On : 10 Aug 2021 1:23
Operator : JU/CG
Sample : M3291-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

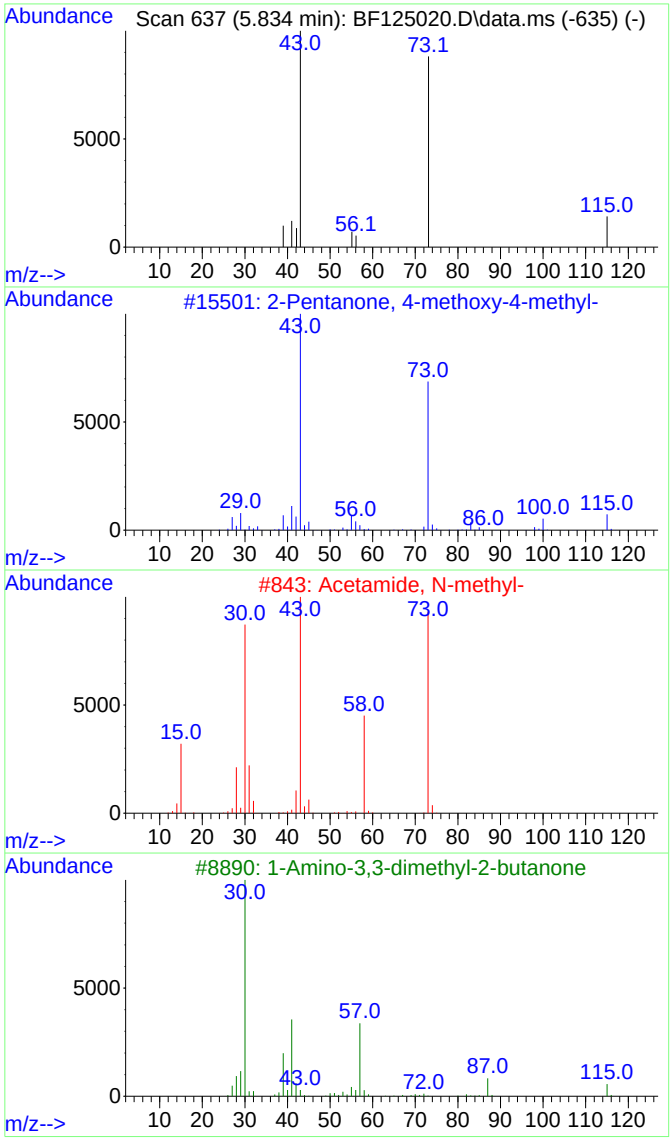
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

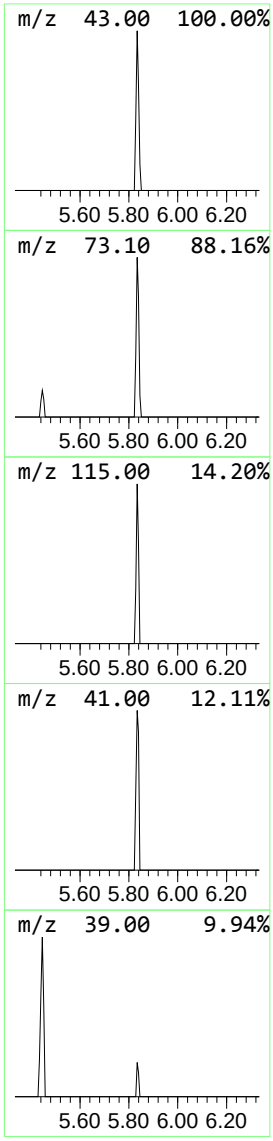
****

Peak Number 2 unknown5.834 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.834	8.77 ng	11935	1,4-Dichlorobenzene-d4	6.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	9
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	5
3	1-Amino-3,3-dimethyl-2-butanone	115	C6H13NO	082962-91-2	4
4	N-Ethylformamide	73	C3H7NO	000627-45-2	4
5	Acetamide, N-(2-methylpropyl)-	115	C6H13NO	001540-94-9	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080921\
Data File : BF125020.D
Acq On : 10 Aug 2021 1:23
Operator : JU/CG
Sample : M3291-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-1

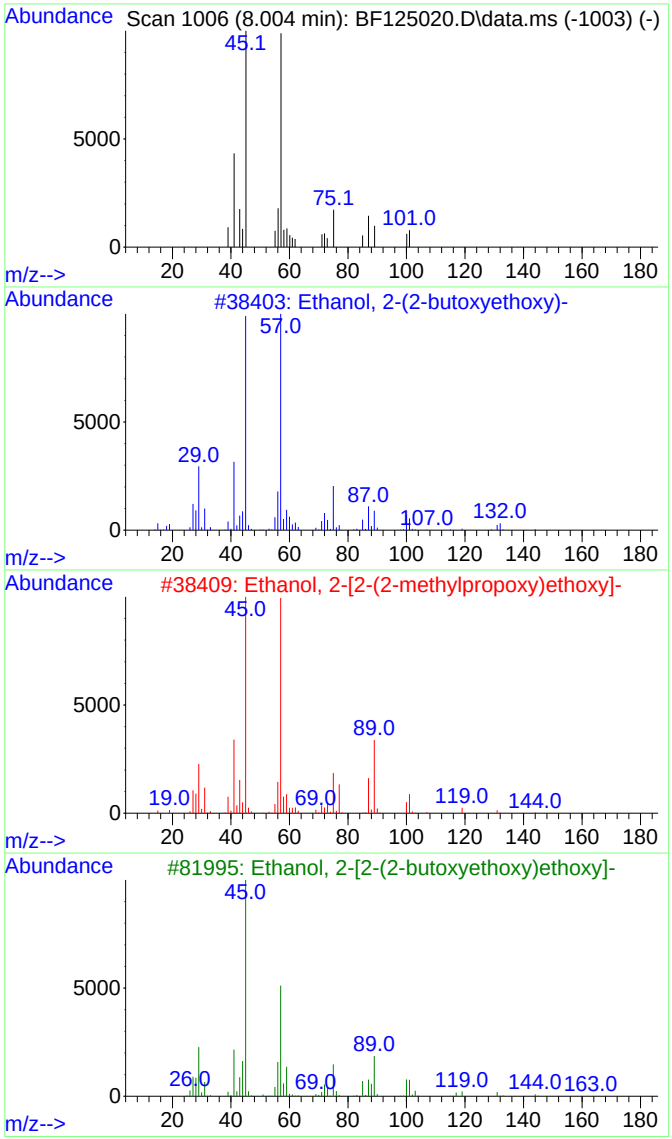
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

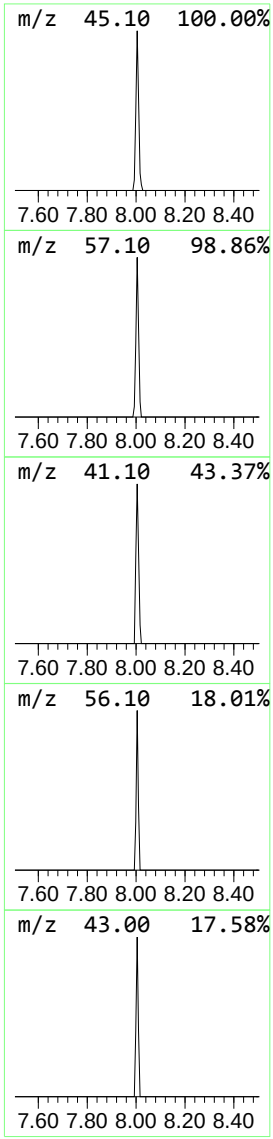
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.004	14.44 ng	23933	Naphthalene-d8	8.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
3	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	50
4	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	40
5	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080921\
Data File : BF125020.D
Acq On : 10 Aug 2021 1:23
Operator : JU/CG
Sample : M3291-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

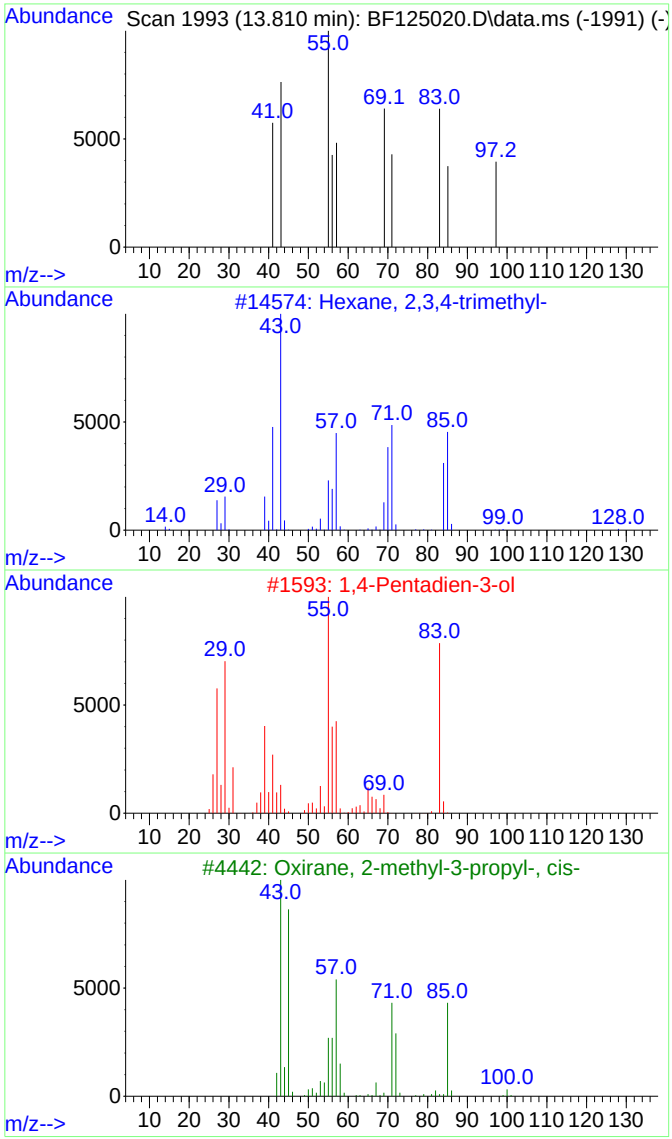
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

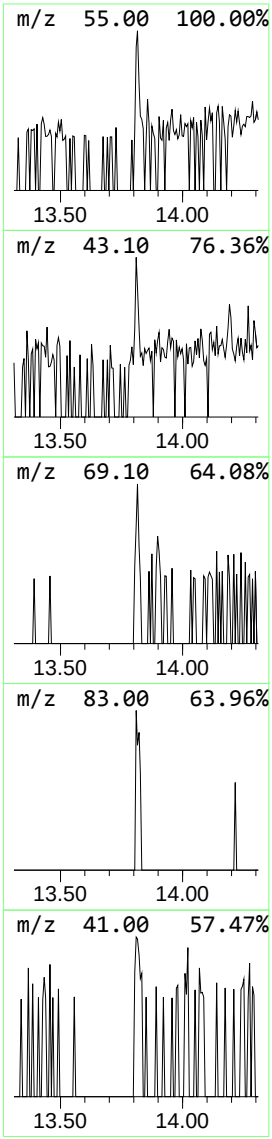
****

Peak Number 4 unknown13.810 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.810	4.09 ng	6192	Chrysene-d12	13.980

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	9
2	1,4-Pentadien-3-ol	84	C5H8O	000922-65-6	9
3	Oxirane, 2-methyl-3-propyl-, cis-	100	C6H12O	006124-90-9	9
4	1,5-Pentanediol, 3-methyl-	118	C6H14O2	004457-71-0	9
5	Pentane, 2-chloro-2-methyl-	120	C6H13Cl	004325-48-8	8





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080921\
Data File : BF125020.D
Acq On : 10 Aug 2021 1:23
Operator : JU/CG
Sample : M3291-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

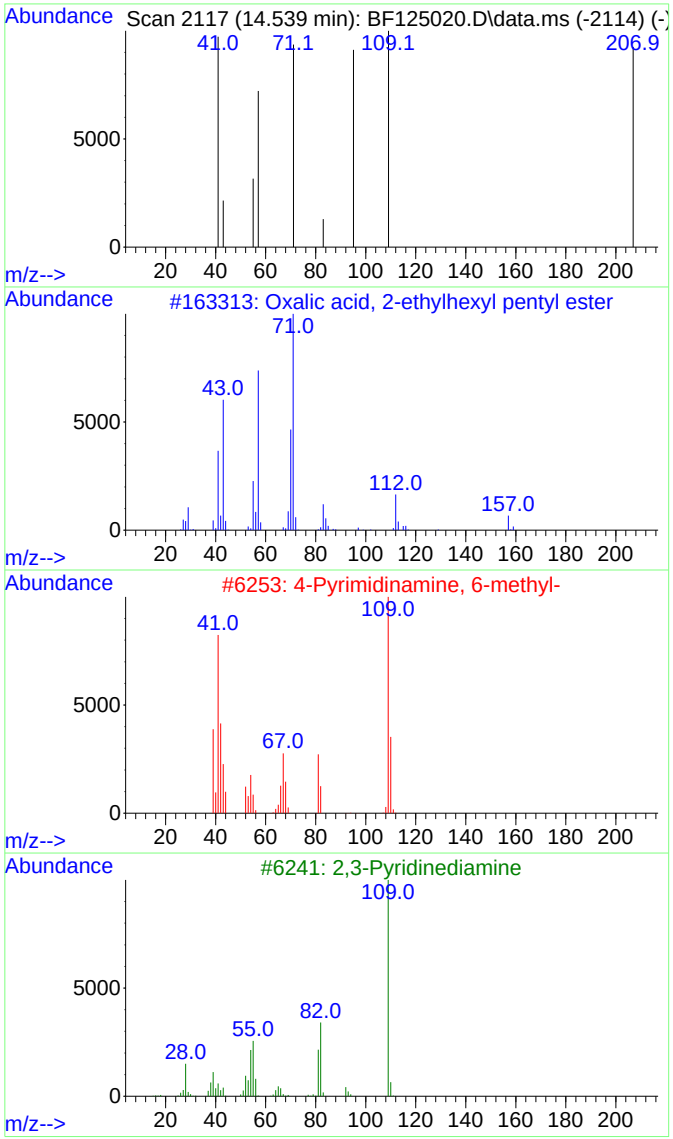
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

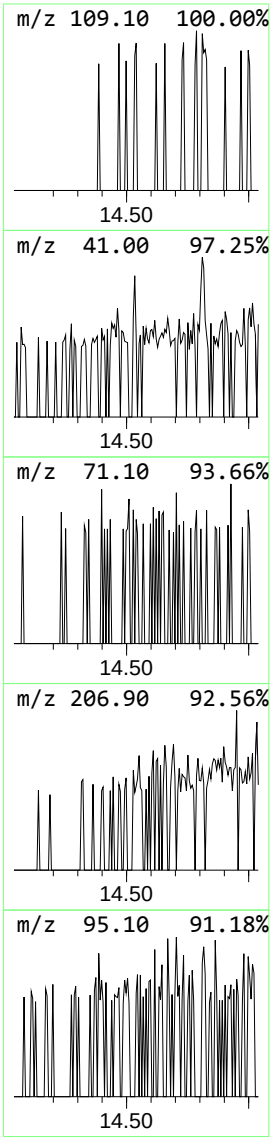
****

Peak Number 5 unknown14.539 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.539	2.25 ng	3406	Chrysene-d12	13.980

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, 2-ethylhexyl pentyl...	272	C15H28O4	1000309-38-7	9
2	4-Pyrimidinamine, 6-methyl-	109	C5H7N3	003435-28-7	4
3	2,3-Pyridinediamine	109	C5H7N3	000452-58-4	4
4	2-Propenamide	71	C3H5NO	000079-06-1	4
5	3-Thiophenecarbonitrile	109	C5H3NS	001641-09-4	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080921\
Data File : BF125020.D
Acq On : 10 Aug 2021 1:23
Operator : JU/CG
Sample : M3291-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

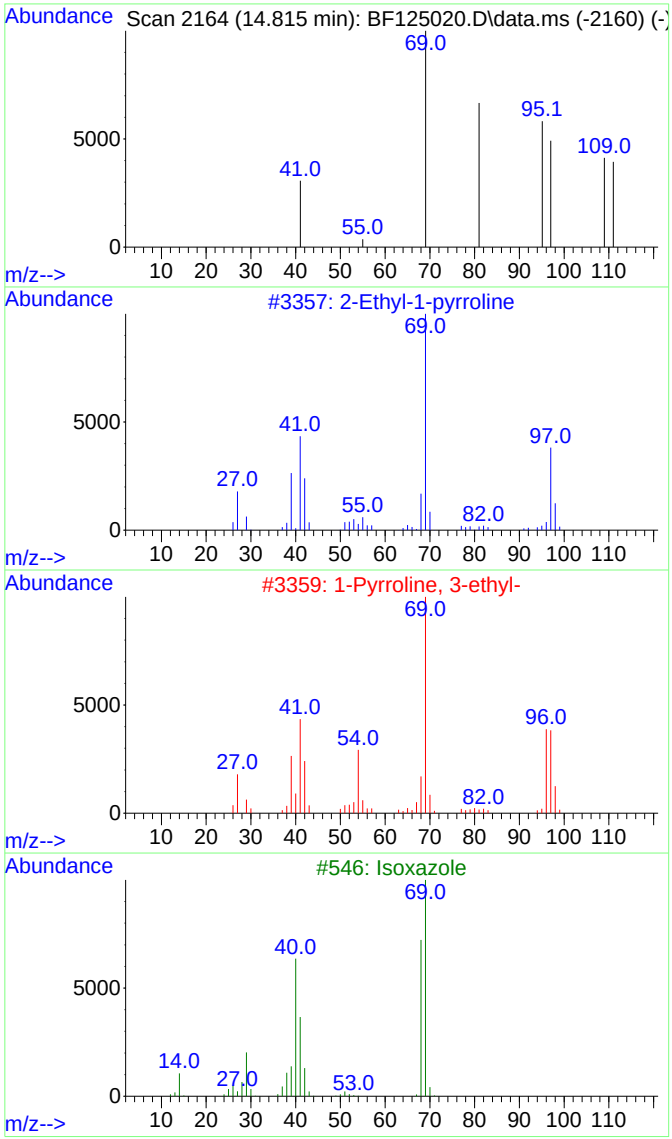
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

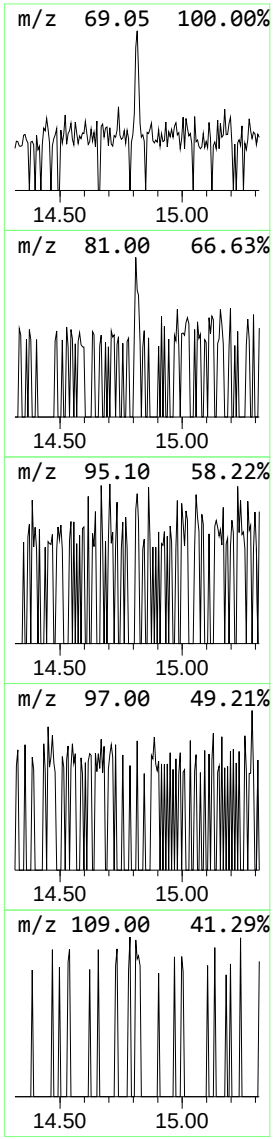
****

Peak Number 6 unknown14.816 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.816	3.27 ng	4115	Perylene-d12	15.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Ethyl-1-pyrroline	97	C6H11N	1000422-81-4	5
2	1-Pyrroline, 3-ethyl-	97	C6H11N	1000073-06-0	5
3	Isoxazole	69	C3H3NO	000288-14-2	3
4	Oxazole	69	C3H3NO	000288-42-6	3
5	1H-Pyrrole-2,5-dione	97	C4H3NO2	000541-59-3	3





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080921\
Data File : BF125020.D
Acq On : 10 Aug 2021 1:23
Operator : JU/CG
Sample : M3291-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

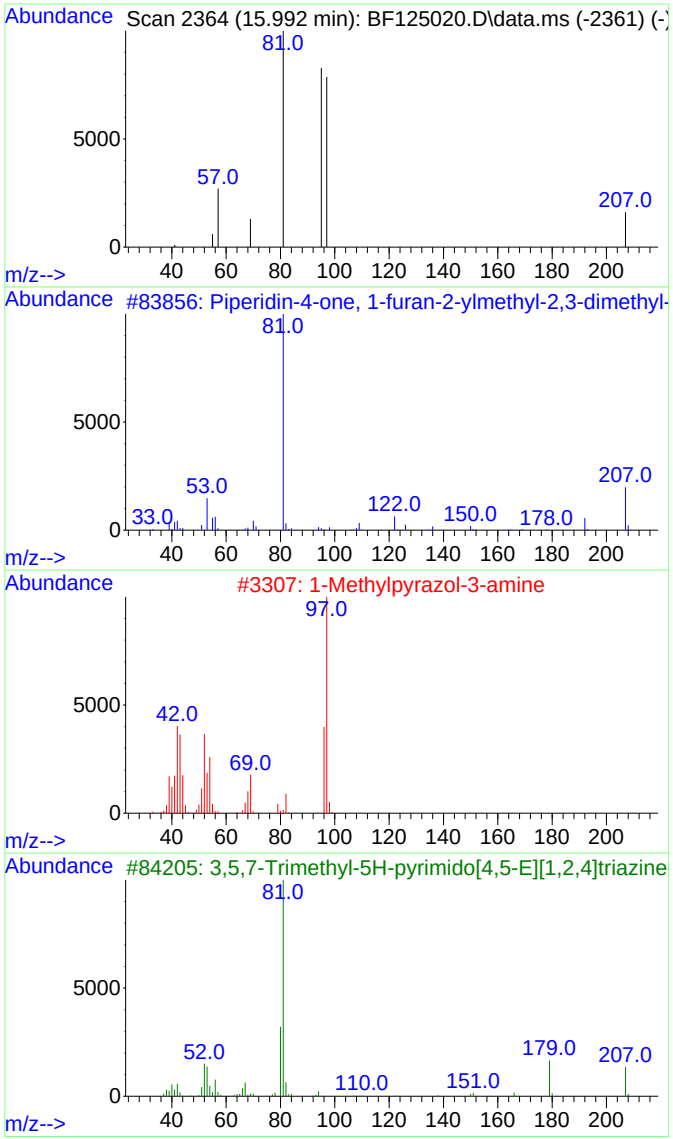
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****

Peak Number 7 unknown15.992 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.992	2.17 ng	2728	Perylene-d12	15.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Piperidin-4-one, 1-furan-2-ylmet...	207	C12H17NO2	1000303-70-3	7
2	1-Methylpyrazol-3-amine	97	C4H7N3	001904-31-0	4
3	3,5,7-Trimethyl-5H-pyrimido[4,5-...	207	C8H9N5O2	1000300-44-3	4
4	Pyridine, 3-fluoro-	97	C5H4FN	000372-47-4	4
5	Aminopyrazine	95	C4H5N3	005049-61-6	4



Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080921\
Data File : BF125020.D
Acq On : 10 Aug 2021 1:23
Operator : JU/CG
Sample : M3291-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	5.040	55.5	ng	75477	1	6.822	27215	20.0
unknown5.834	5.834	8.8	ng	11935	1	6.822	27215	20.0
Ethanol, 2-(2-b...	8.004	14.4	ng	23933	2	8.104	33145	20.0
unknown13.810	13.810	4.1	ng	6192	5	13.980	30292	20.0
unknown14.539	14.539	2.3	ng	3406	5	13.980	30292	20.0
unknown14.816	14.816	3.3	ng	4115	6	15.439	25167	20.0
unknown15.992	15.992	2.2	ng	2728	6	15.439	25167	20.0