LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016635.D
Acq On : 01 Oct 2021 14:42
Operator : CG/JU
Sample : M3990-06MS
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : S-836-K1-SO-1-1.5-092921MS

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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_N\METHODS\8270-SIM-BN100121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BN016635.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.281	20	22	25	rBV	12430	16663	3.42%	0.189%
2	3.530	46	49	53	rBV	28861	50274	10.33%	0.569%
3	3.594	53	56	64	rVB	15364	29728	6.11%	0.337%
4	3.843	80	83	98	rVB	14392	38678	7.95%	0.438%
5	4.249	125	127	130	rBV	9945	15058	3.09%	0.170%
6	4.830	186	190	204	rVB	204377	317837	65.30%	3.599%
7	5.051	211	214	221	rVB	4029	8524	1.75%	0.097%
8	5.291	236	240	249	rVB	25826	45154	9.28%	0.511%
9	5.761	288	291	297	rVB	4523	8899	1.83%	0.101%
10	6.665	385	389	397	rVB	7237	14008	2.88%	0.159%
11	6.831	404	407	418	rVB2	28576	66269	13.62%	0.750%
12	6.988	420	424	430	rBV	11786	23049	4.74%	0.261%
13	7.080	430	434	442	rVB	38474	64485	13.25%	0.730%
14	7.218	445	449	450	rBV	11853	21185	4.35%	0.240%
15	7.532	480	483	490	rVV2	7227	14541	2.99%	0.165%
16	7.642	491	495	501	rVV2	56336	107948	22.18%	1.222%
17	7.707	501	502	507	rVB	7121	7945	1.63%	0.090%
18	7.873	517	520	525	rVB2	3427	7171	1.47%	0.081%
19	7.983	529	532	540	rVB	6773	14042	2.89%	0.159%
20	8.177	549	553	559	rVB	4043	9908	2.04%	0.112%
21	8.306	565	567	569	rVB2	8826	8827	1.81%	0.100%
22	8.442	569	578	582	rBV2	39336	96009	19.73%	1.087%
23	8.696	595	598	602	rBV	4434	7967	1.64%	0.090%
24	8.784	602	605	607	rVV	32827	64820	13.32%	0.734%
25	8.822	607	608	613	rVV	27873	40576	8.34%	0.459%
26	8.911	613	615	617	rVV	3285	6800	1.40%	0.077%
27	8.949	617	618	622	rVB	6443	9069	1.86%	0.103%
28	9.342	646	649	656	rVB	47466	76927	15.81%	0.871%
29	9.532	660	664	666	rBV	3979	8172	1.68%	0.093%
30	9.595	666	669	672	rVV	9653	18926	3.89%	0.214%
31	9.646	672	673	678	rVB	4360	7485	1.54%	0.085%
32	9.836	685	688	691	rBV	18729	29042	5.97%	0.329%
33	10.064	703	706	713	rBV2	5333	12801	2.63%	0.145%
34	10.204	713	717	720	rBV	235594	383077	78.71%	4.337%
35	10.407	730	733	735	rBV	98322	170539	35.04%	1.931%
36	10.457	735	737	740	rVV	99599	160073	32.89%	1.812%

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Misc :
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Instrument : BNA_N
ClientSampleId : S-836-K1-SO-1-1.5-092921MS

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	10.584	744	747	754	rVB	13249	28538	5.86%	0.323%
38	10.749	757	760	764	rVB	29319	47120	9.68%	0.534%
39	11.306	801	804	813	rVB	3893	9008	1.85%	0.102%
40	11.709	855	865	889	rBV	14821	25545	5.25%	0.289%
41	12.003	916	931	940	rBV	48907	81011	16.64%	0.917%
42	12.078	940	948	971	rVB	118334	185238	38.06%	2.097%
43	12.301	987	998	1020	rVB	111428	173812	35.71%	1.968%
44	12.695	1056	1059	1062	rBV	16273	26333	5.41%	0.298%
45	12.771	1062	1065	1071	rVB	12531	23495	4.83%	0.266%
46	12.886	1071	1074	1078	rBV2	81869	151822	31.19%	1.719%
47	13.101	1088	1091	1092	rBV	121842	181197	37.23%	2.052%
48	13.139	1092	1094	1096	rVV	76708	131196	26.96%	1.485%
49	13.177	1096	1097	1106	rVV	41435	55879	11.48%	0.633%
50	13.736	1138	1141	1143	rVB	11798	15936	3.27%	0.180%
51	13.850	1148	1150	1153	rVB	18459	27094	5.57%	0.307%
52	13.989	1158	1161	1164	rVB	98382	148848	30.58%	1.685%
53	14.269	1180	1183	1186	rBV	125654	183749	37.75%	2.080%
54	14.332	1186	1188	1191	rVV	149946	210642	43.28%	2.385%
55	14.434	1194	1196	1200	rVV	11983	18746	3.85%	0.212%
56	14.510	1200	1202	1206	rVV3	3129	7631	1.57%	0.086%
57	14.637	1210	1212	1219	rVV2	16334	43283	8.89%	0.490%
58	14.814	1222	1226	1229	rVV2	4844	11514	2.37%	0.130%
59	14.903	1229	1233	1239	rVB3	6644	15258	3.13%	0.173%
60	15.106	1246	1249	1255	rVB	10020	15078	3.10%	0.171%
61	15.322	1263	1266	1270	rBV2	200262	313739	64.46%	3.552%
62	15.537	1280	1283	1287	rBV	33685	55372	11.38%	0.627%
63	15.613	1287	1289	1295	rVV2	38048	66548	13.67%	0.753%
64	15.715	1295	1297	1299	rVV	13952	20829	4.28%	0.236%
65	15.766	1299	1301	1305	rVB2	11927	18611	3.82%	0.211%
66	15.969	1315	1317	1322	rVB3	3722	9375	1.93%	0.106%
67	16.226	1334	1338	1343	rBV2	56127	89248	18.34%	1.010%
68	16.324	1343	1346	1353	rVB	41153	68108	13.99%	0.771%
69	16.506	1358	1361	1366	rVV	26037	40760	8.37%	0.461%
70	16.677	1372	1375	1384	rVB	32201	51560	10.59%	0.584%
71	16.835	1384	1388	1393	rVB2	5949	10978	2.26%	0.124%
72	17.017	1400	1403	1405	rBV	96095	154950	31.84%	1.754%
73	17.066	1405	1407	1410	rVV	134987	193545	39.77%	2.191%
74	17.151	1411	1414	1419	rVV	117881	182525	37.50%	2.067%
75	17.431	1434	1437	1446	rBV	88298	130622	26.84%	1.479%
76	18.015	1482	1485	1497	rVB	9353	13819	2.84%	0.156%

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Misc :
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Instrument : BNA_N
ClientSampleId : S-836-K1-SO-1-1.5-092921MS

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : OFF Filtering: 5
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Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
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77	18.909	1661	1665	1675	rVB	10349	11748	2.41%	0.133%
78	19.063	1687	1696	1699	rBV	108552	153666	31.57%	1.740%
79	19.093	1699	1702	1727	rVV	183421	243044	49.94%	2.752%
80	19.460	1766	1776	1797	rVB	187266	251536	51.68%	2.848%
81	19.678	1813	1820	1838	rBV	87662	107200	22.03%	1.214%
82	20.378	1918	1921	1924	rBV	88548	103979	21.36%	1.177%
83	20.972	1974	1977	1981	rVB	17882	27024	5.55%	0.306%
84	21.164	1992	1995	1998	rBV	142569	199499	40.99%	2.259%
85	21.217	1998	2000	2003	rVV2	219353	417279	85.74%	4.725%
86	21.270	2003	2005	2008	rVB	178115	230701	47.40%	2.612%
87	21.854	2057	2060	2067	rBV2	5064	13950	2.87%	0.158%
88	22.056	2076	2079	2082	rBV	117990	161053	33.09%	1.823%
89	22.109	2082	2084	2089	rVB	23046	33117	6.80%	0.375%
90	22.311	2100	2103	2107	rBV2	6876	15867	3.26%	0.180%
91	22.395	2108	2111	2113	rVB2	7489	10906	2.24%	0.123%
92	22.803	2217	2228	2235	rBV	131244	220636	45.33%	2.498%
93	22.848	2235	2241	2271	rVB	126921	230812	47.42%	2.613%
94	23.382	2385	2397	2414	rBV	105856	201878	41.48%	2.286%
95	23.481	2415	2426	2454	rVB	97860	197331	40.54%	2.234%
96	24.083	2593	2602	2615	rVB2	4899	9342	1.92%	0.106%
97	24.172	2617	2628	2651	rBV	12988	36812	7.56%	0.417%
98	24.853	2820	2827	2843	rVB	3376	7183	1.48%	0.081%
99	25.771	3071	3095	3128	rBV4	136695	486705	100.00%	5.511%
100	26.452	3273	3294	3333	rBV	74127	239817	49.27%	2.715%

Sum of corrected areas: 8832123

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
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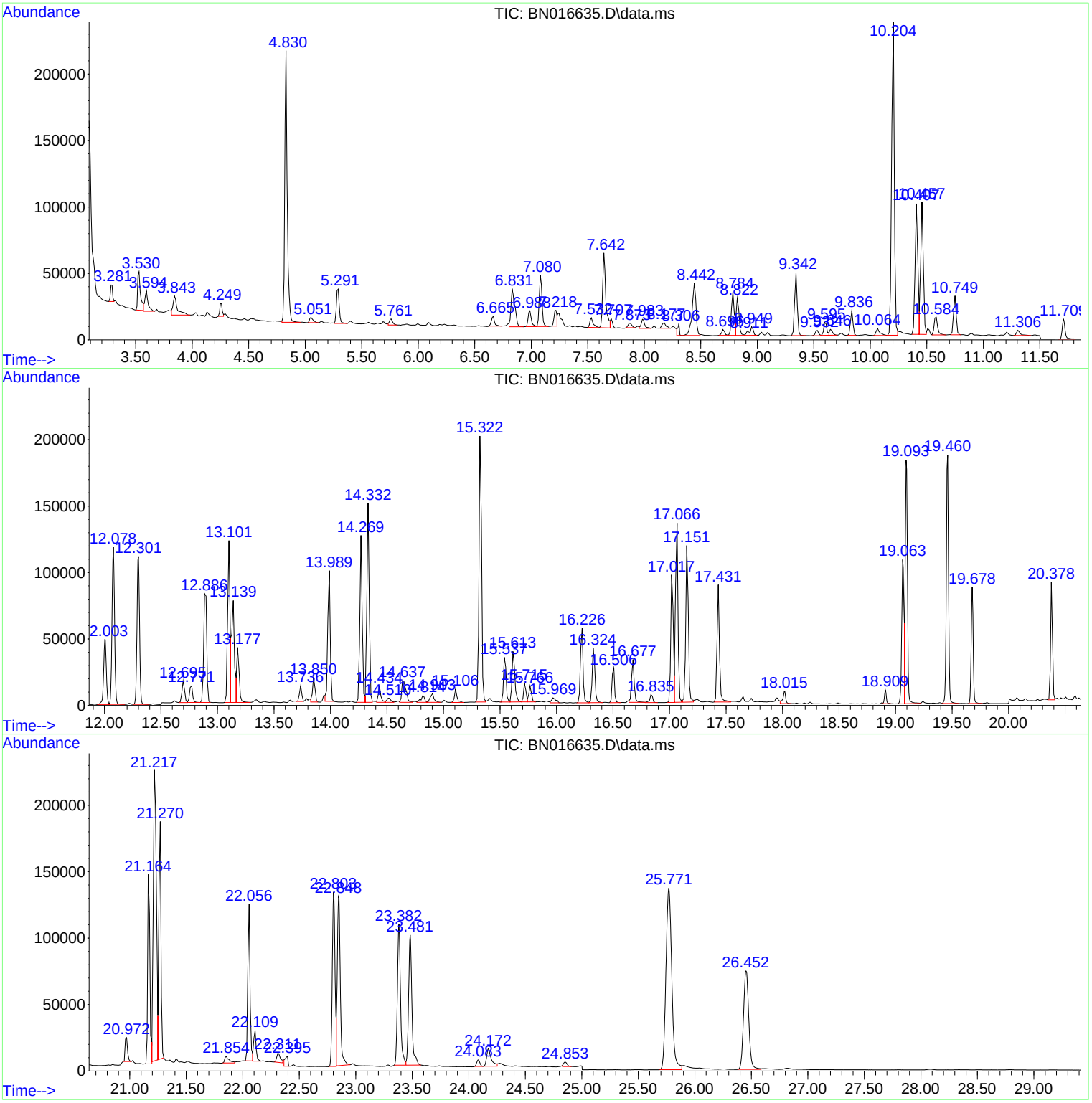
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-836-K1-SO-1-1.5-092921MS

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.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_N\Data\BN100121\
Data File : BN016635.D
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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_N
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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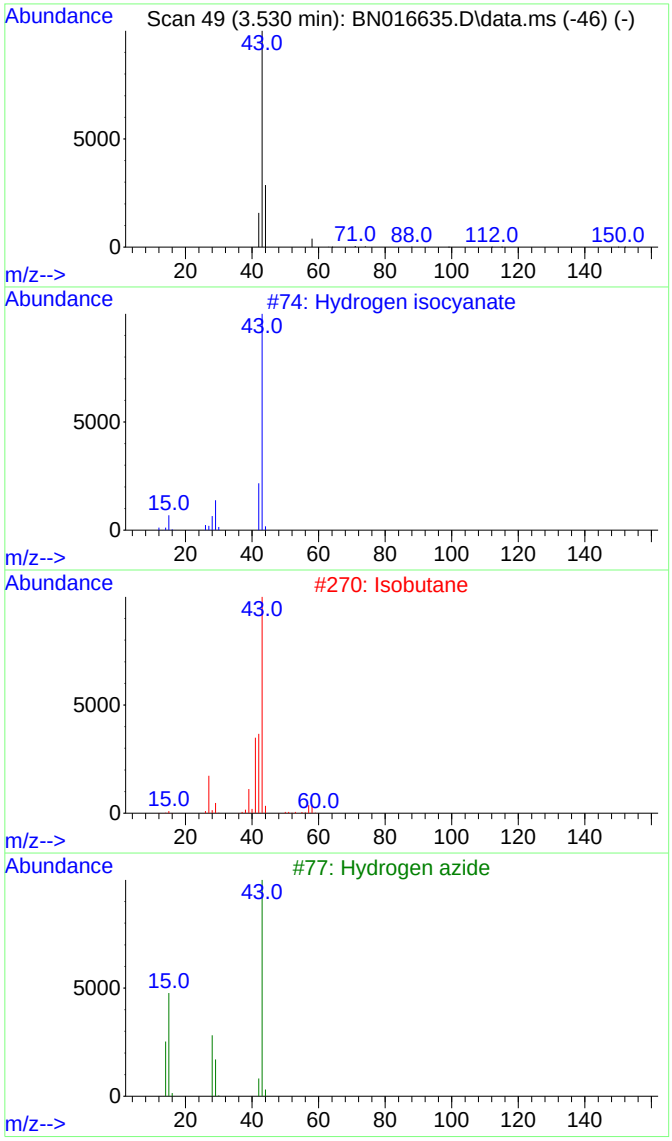
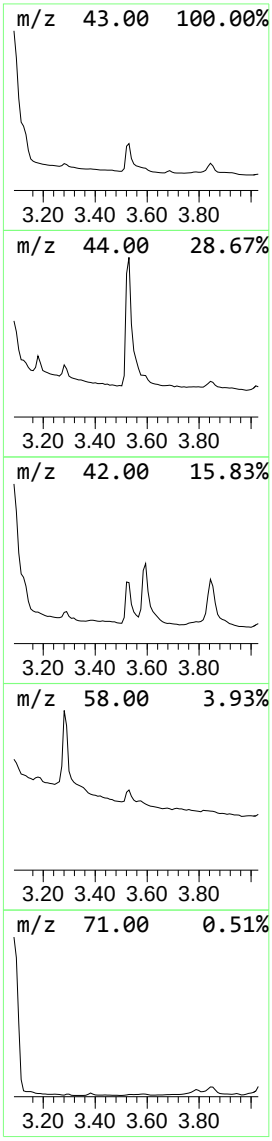
****

Peak Number 1 Hydrogen isocyanate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.530	0.19 ng	50274	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrogen isocyanate	43	CHNO	000075-13-8	3
2	Isobutane	58	C4H10	000075-28-5	3
3	Hydrogen azide	43	HN3	007782-79-8	3
4	1-Butanol	74	C4H10O	000071-36-3	2
5	1,4-Butanediamine	88	C4H12N2	000110-60-1	2





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016635.D
Acq On : 01 Oct 2021 14:42
Operator : CG/JU
Sample : M3990-06MS
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-836-K1-SO-1-1.5-092921MS

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

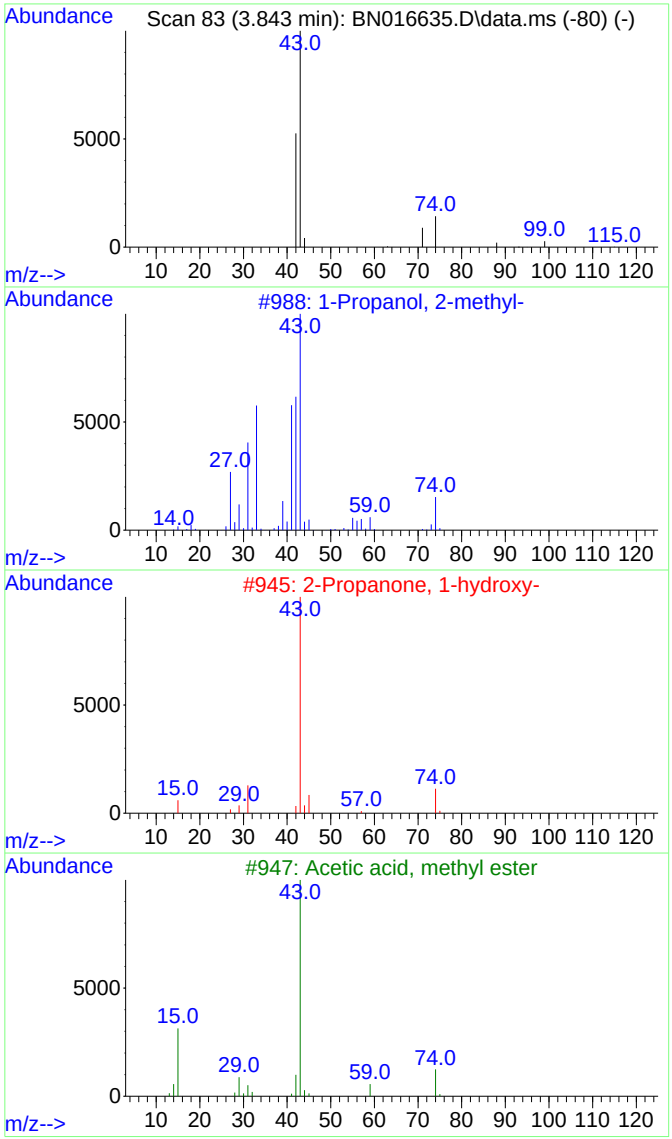
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

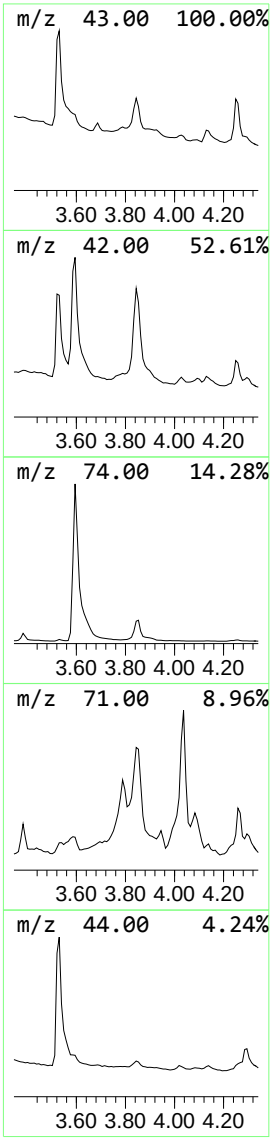
****

Peak Number 2 1-Propanol, 2-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.843	0.14 ng	38678	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
2	2-Propanone, 1-hydroxy-	74	C3H6O2	000116-09-6	4
3	Acetic acid, methyl ester	74	C3H6O2	000079-20-9	4
4	Acetic acid, hydrazide	74	C2H6N2O	001068-57-1	4
5	Cyanamide	42	CH2N2	000420-04-2	3





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

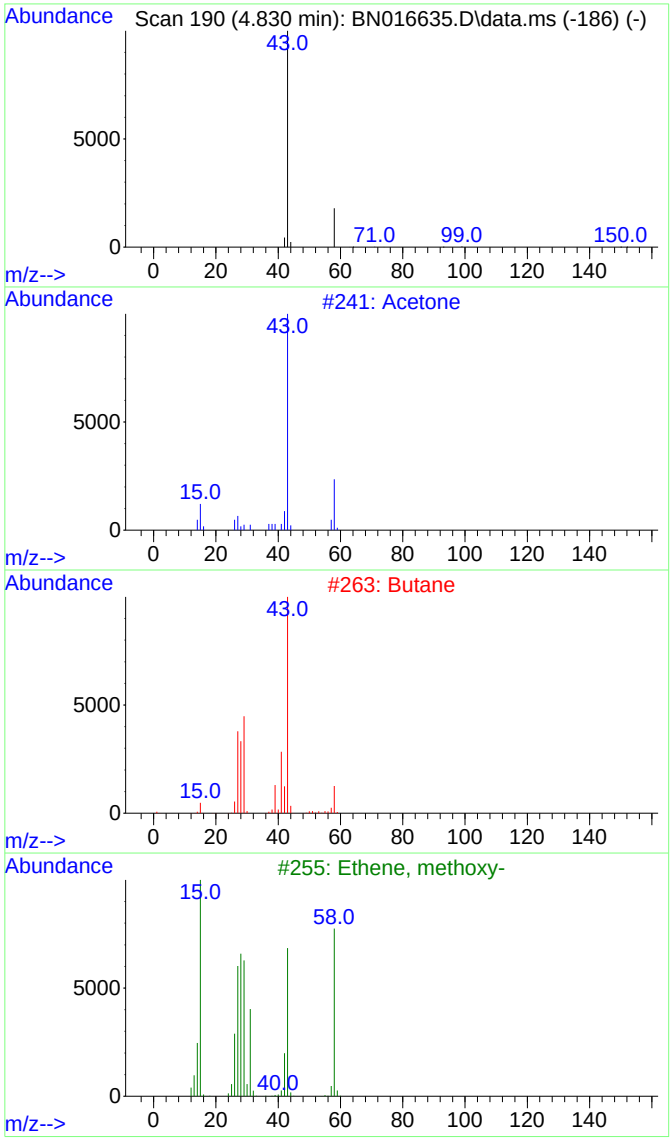
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

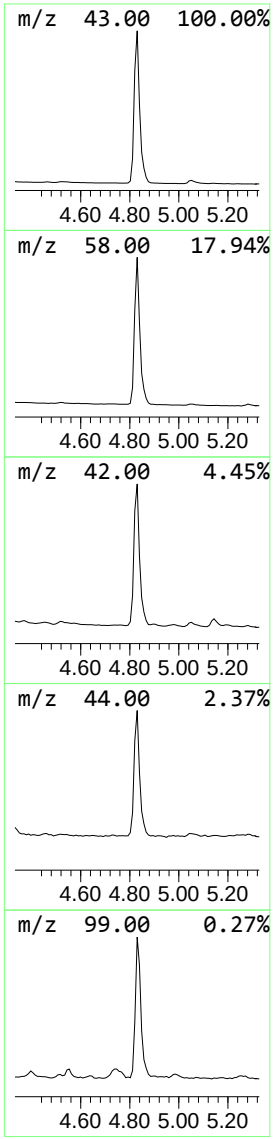
****

Peak Number 3 Acetone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.830	1.18 ng	317837	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetone	58	C3H6O	000067-64-1	4
2	Butane	58	C4H10	000106-97-8	4
3	Ethene, methoxy-	58	C3H6O	000107-25-5	3
4	Diazene, dimethyl-	58	C2H6N2	000503-28-6	3
5	Hydrogen isocyanate	43	CHNO	000075-13-8	2





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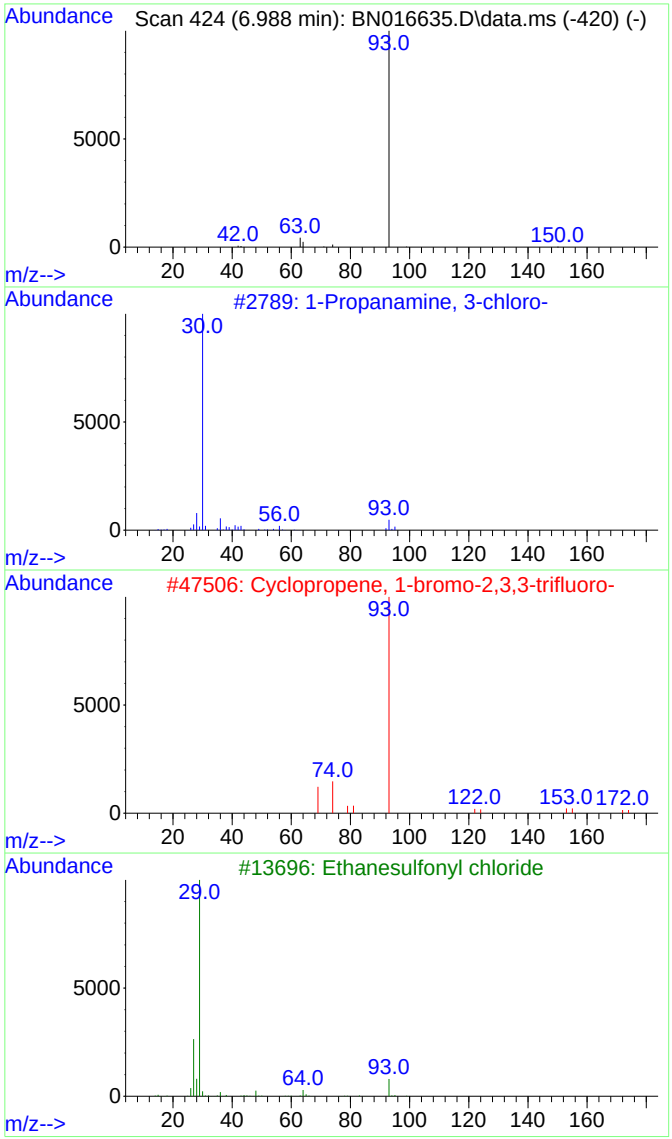
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

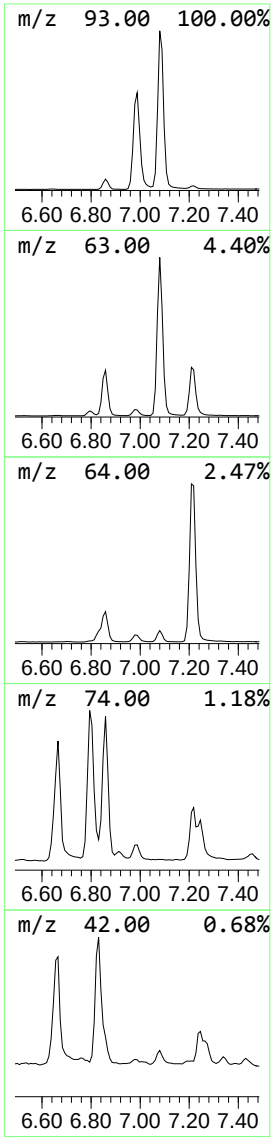
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Propanamine, 3-chloro- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.988	0.09 ng	23049	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanamine, 3-chloro-	93	C3H8ClN	014753-26-5	1
2	Cyclopropene, 1-bromo-2,3,3-trif...	172	C3BrF3	029777-44-4	1
3	Ethanesulfonyl chloride	128	C2H5ClO2S	000594-44-5	1
4	Carbonochloridic acid, ethyl ester	108	C3H5ClO2	000541-41-3	1
5	Ethenesulfonyl chloride	126	C2H3ClO2S	006608-47-5	1





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Data File : BN016635.D
Acq On : 01 Oct 2021 14:42
Operator : CG/JU
Sample : M3990-06MS
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-836-K1-SO-1-1.5-092921MS

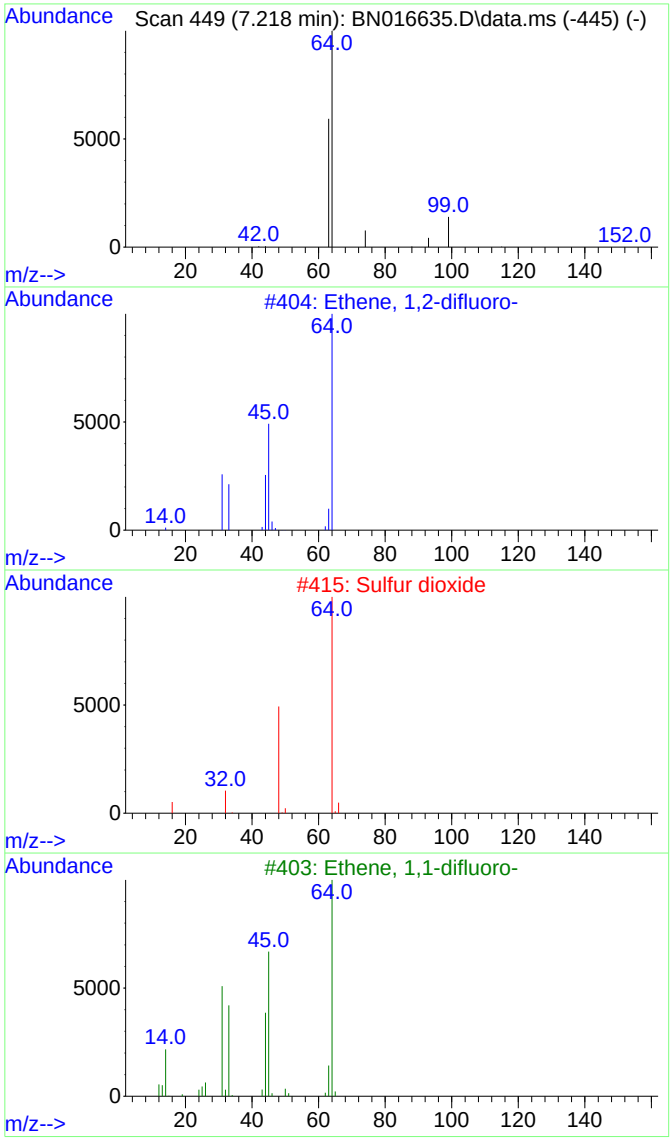
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

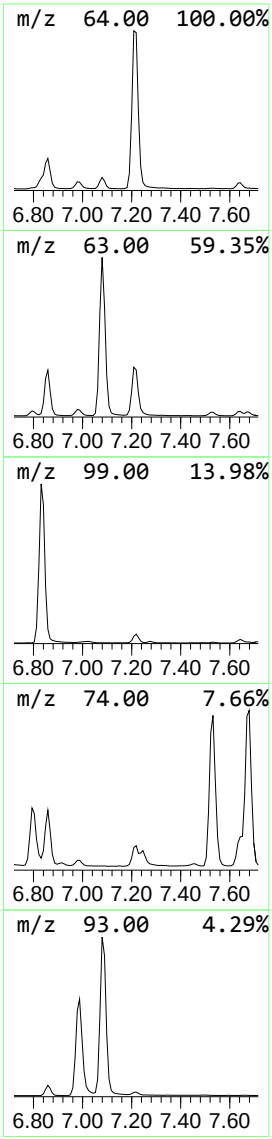
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Ethene, 1,2-difluoro- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.218	0.08 ng	21185	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	3
2	Sulfur dioxide	64	O2S	007446-09-5	3
3	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	3
4	Ethyl Chloride	64	C2H5Cl	000075-00-3	3
5	(S)-(-)-2-Chloropropionic acid	108	C3H5ClO2	029617-66-1	2





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Acq On : 01 Oct 2021 14:42
Operator : CG/JU
Sample : M3990-06MS
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
S-836-K1-SO-1-1.5-092921MS

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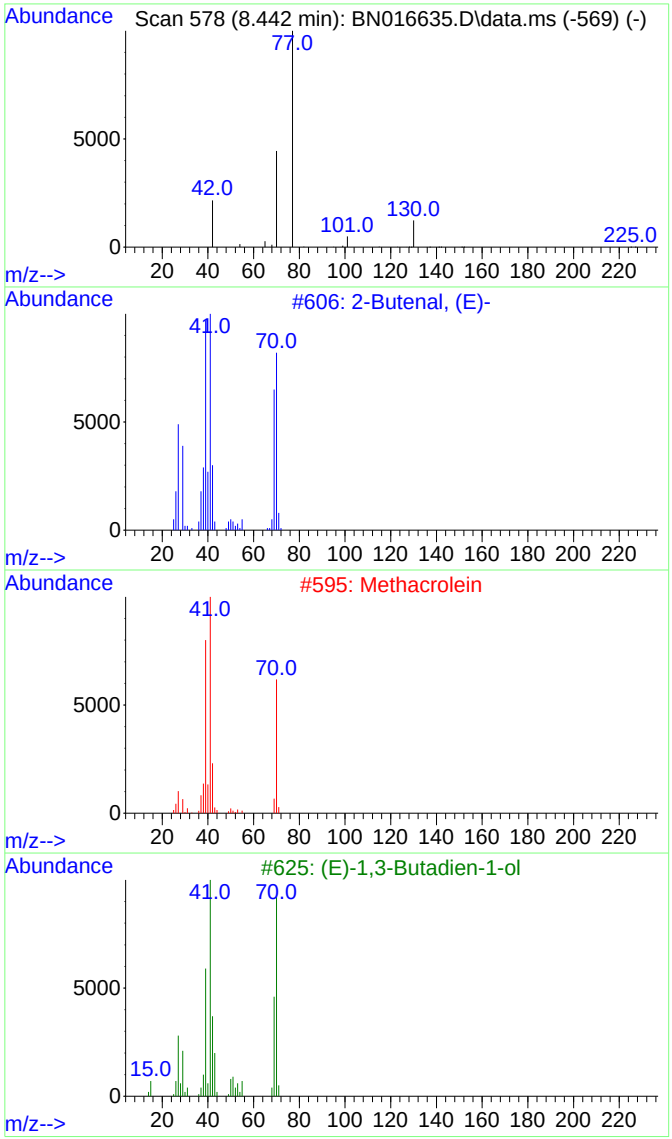
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

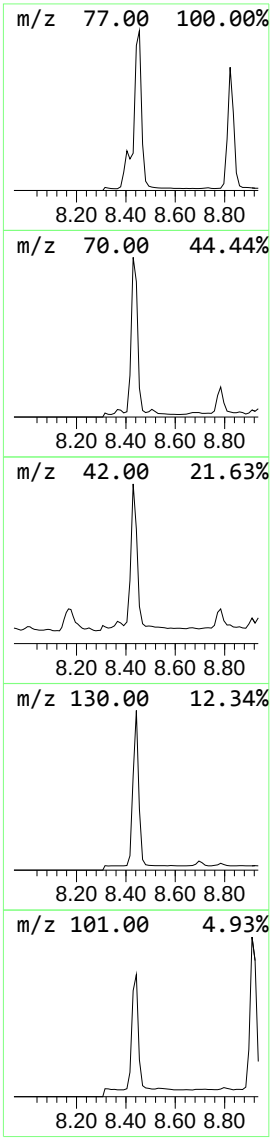
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 2-Butenal, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.442	0.36 ng	96009	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenal, (E)-	70	C4H6O	000123-73-9	4
2	Methacrolein	70	C4H6O	000078-85-3	4
3	(E)-1,3-Butadien-1-ol	70	C4H6O	070411-98-2	4
4	Carbonic acid, methyl tetradecyl...	272	C16H32O3	1000314-62-5	4
5	Furan, 2,3-dihydro-	70	C4H6O	001191-99-7	3





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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-836-K1-SO-1-1.5-092921MS

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

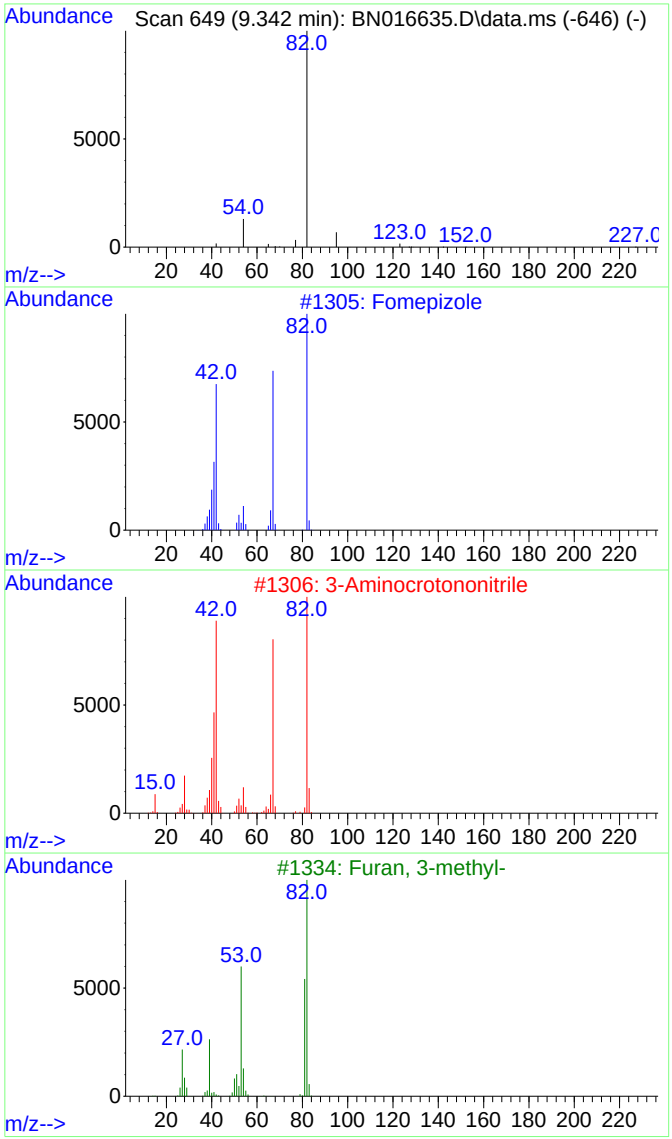
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

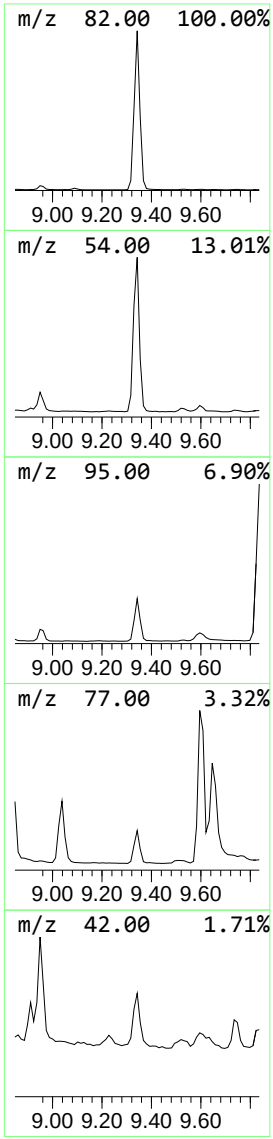
****

Peak Number 7 Fomepizole Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.342	0.18 ng	76927	Naphthalene-d8	10.406

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fomepizole	82	C4H6N2	007554-65-6	5
2	3-Aminocrotononitrile	82	C4H6N2	001118-61-2	4
3	Furan, 3-methyl-	82	C5H6O	000930-27-8	4
4	1H-Pyrazole, 1-methyl-	82	C4H6N2	000930-36-9	4
5	Furan, 2-methyl-	82	C5H6O	000534-22-5	4





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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
S-836-K1-SO-1-1.5-092921MS

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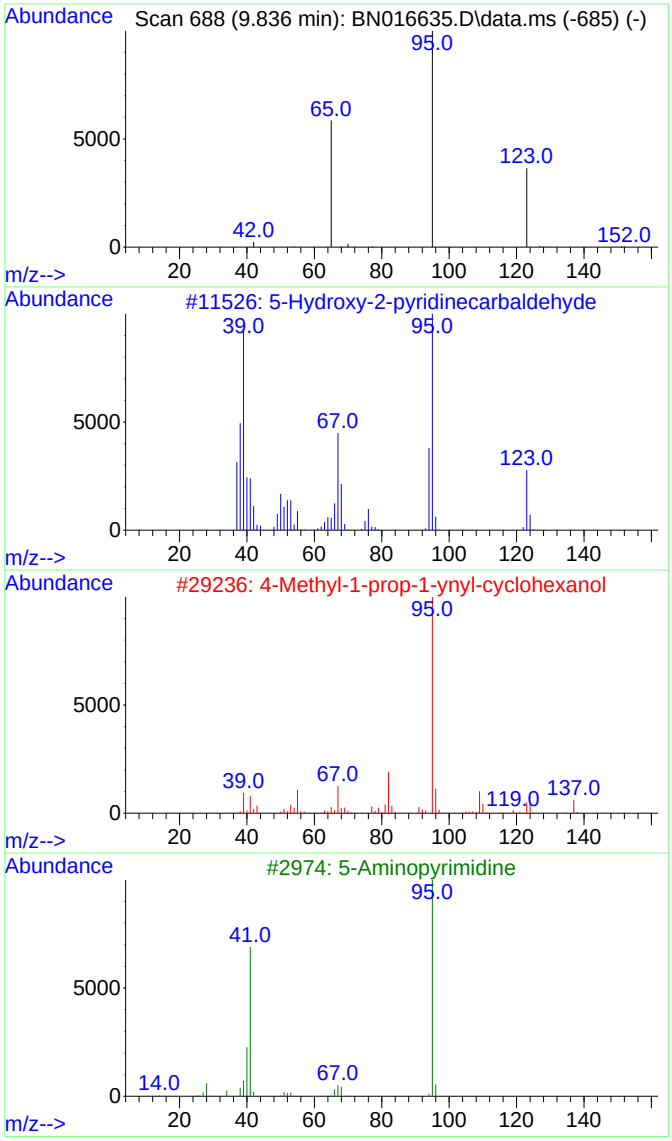
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

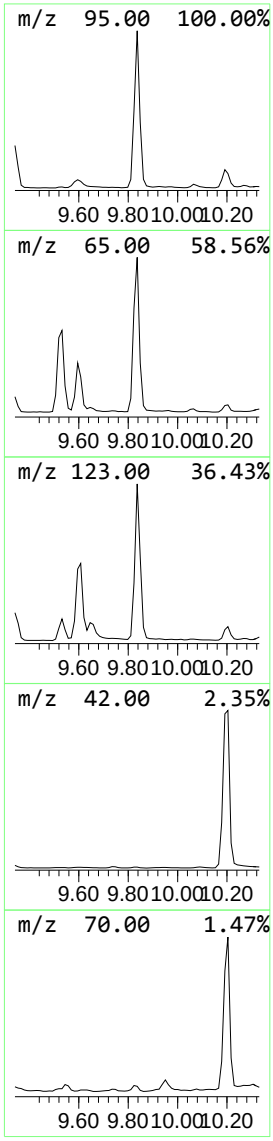
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 5-Hydroxy-2-pyridinecarbald... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.836	0.07 ng	29042	Naphthalene-d8	10.406

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Hydroxy-2-pyridinecarbaldehyde	123	C6H5NO2	031191-08-9	5
2	4-Methyl-1-prop-1-ynyl-cyclohexanol	152	C10H16O	1000362-94-7	3
3	5-Aminopyrimidine	95	C4H5N3	000591-55-9	3
4	2-Pyrimidinamine	95	C4H5N3	000109-12-6	2
5	Pyridine, 1-oxide	95	C5H5NO	000694-59-7	2





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Sample : M3990-06MS
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
S-836-K1-SO-1-1.5-092921MS

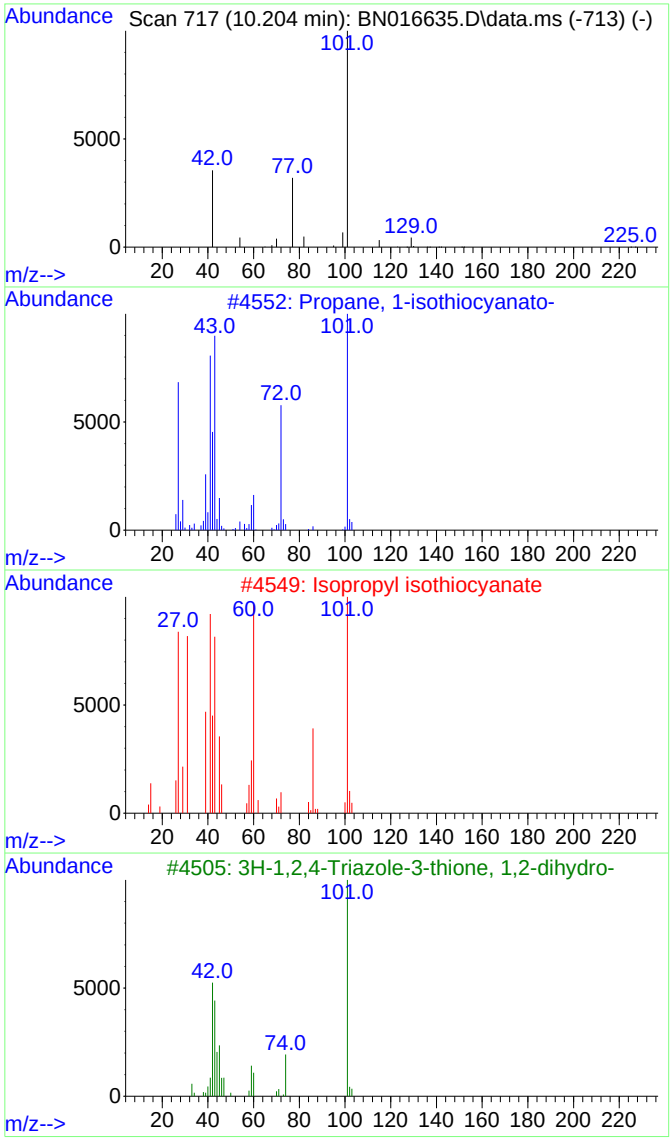
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

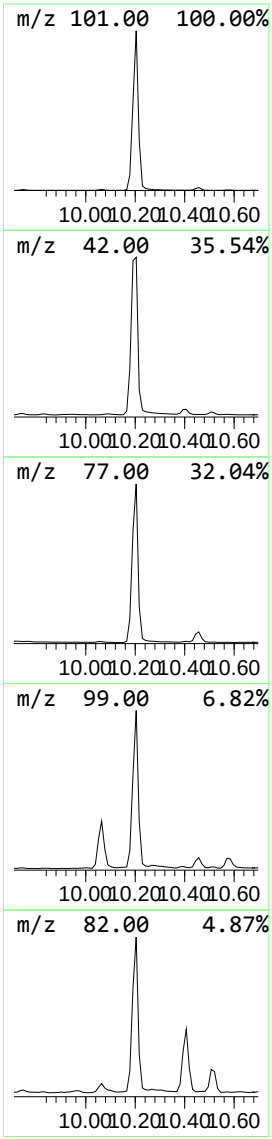
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Propane, 1-isothiocyanato- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.204	0.90 ng	383077	Naphthalene-d8	10.406

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	5
2	Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	5
3	3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	5
4	2-Pyrrolidinethione	101	C4H7NS	002295-35-4	4
5	3-Aminopropionitrile	70	C3H6N2	000151-18-8	4





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Misc :
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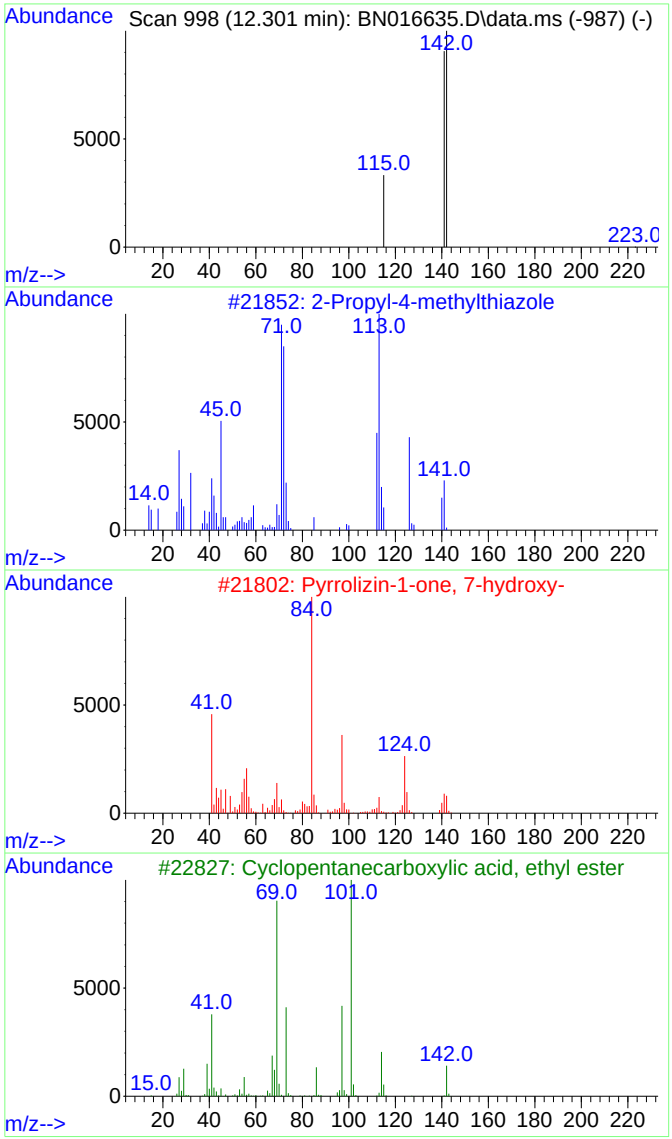
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

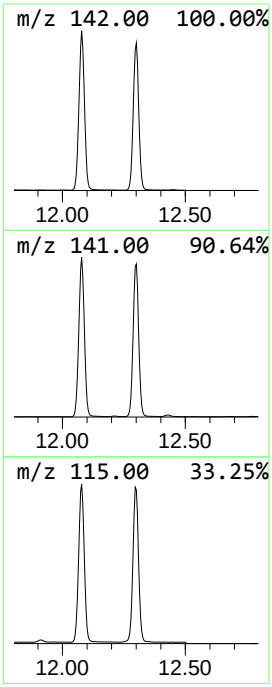
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 2-Propyl-4-methylthiazole Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.301	0.41 ng	173812	Naphthalene-d8	10.406

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propyl-4-methylthiazole	141	C7H11NS	052414-87-6	4
2	Pyrrolizin-1-one, 7-hydroxy-	141	C7H11NO2	1000125-96-2	3
3	Cyclopentanecarboxylic acid, eth...	142	C8H14O2	1000375-86-4	3
4	2-Propionylthiazole	141	C6H7NOS	043039-98-1	3
5	2,4(1H,3H)-Pyrimidinedione, 6-am...	141	C5H7N3O2	002434-53-9	2





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

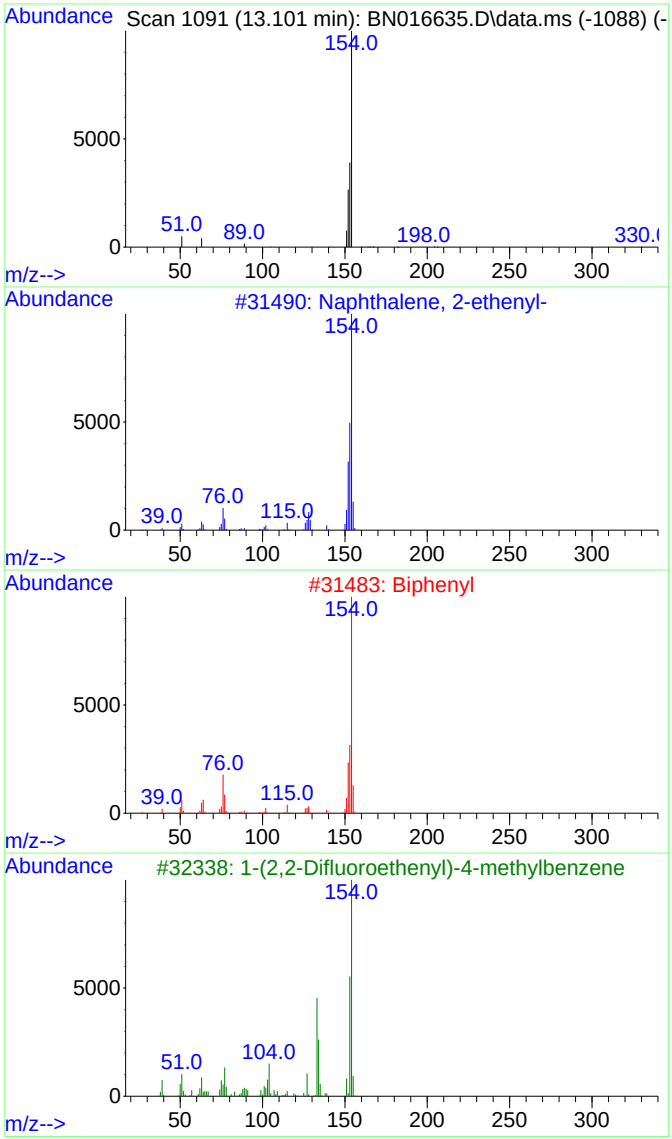
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

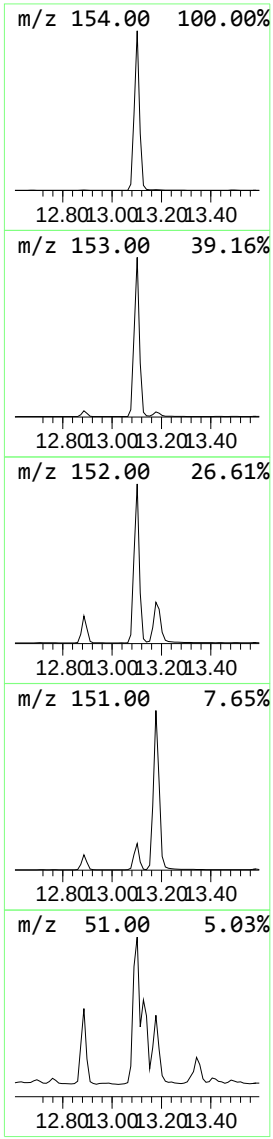
****

Peak Number 11 Naphthalene, 2-ethenyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.101	0.39 ng	181197	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	50
2	Biphenyl	154	C12H10	000092-52-4	45
3	1-(2,2-Difluoroethenyl)-4-methyl...	154	C9H8F2	1000305-64-2	9
4	Octahydro-1H-pyrido(1,2-c)pyrimi...	154	C8H14N2O	015932-63-5	5
5	Furane-2-carboxaldehyde, iminose...	152	C6H8N4O	004353-50-8	5





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Misc :
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Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

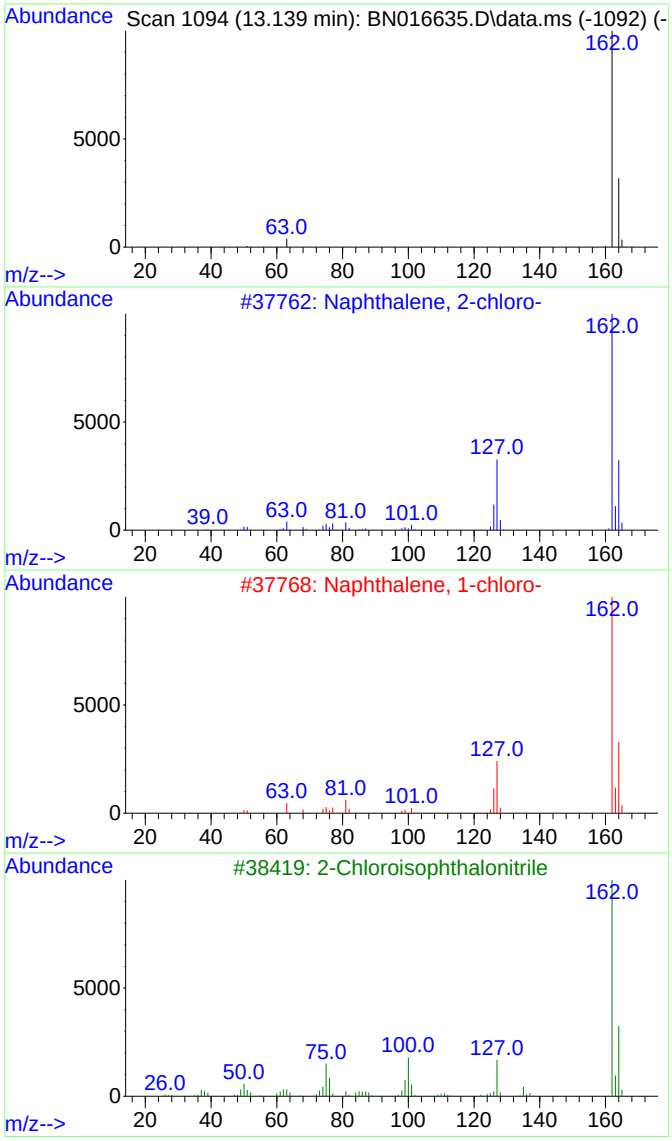
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

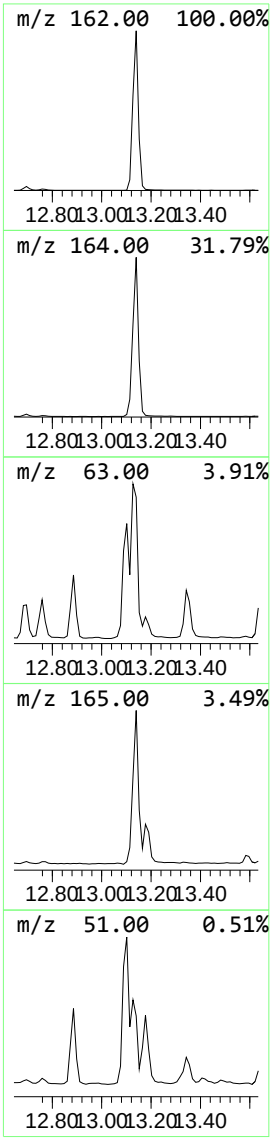
****

Peak Number 12 Naphthalene, 2-chloro- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.139	0.29 ng	131196	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-chloro-	162	C10H7Cl	000091-58-7	74
2	Naphthalene, 1-chloro-	162	C10H7Cl	000090-13-1	74
3	2-Chloroisophthalonitrile	162	C8H3ClN2	028442-78-6	7
4	3-Chlorophthalonitrile	162	C8H3ClN2	076241-79-7	7
5	3-Chloro-4-fluorothiophenol	162	C6H4ClFS	060811-23-6	5





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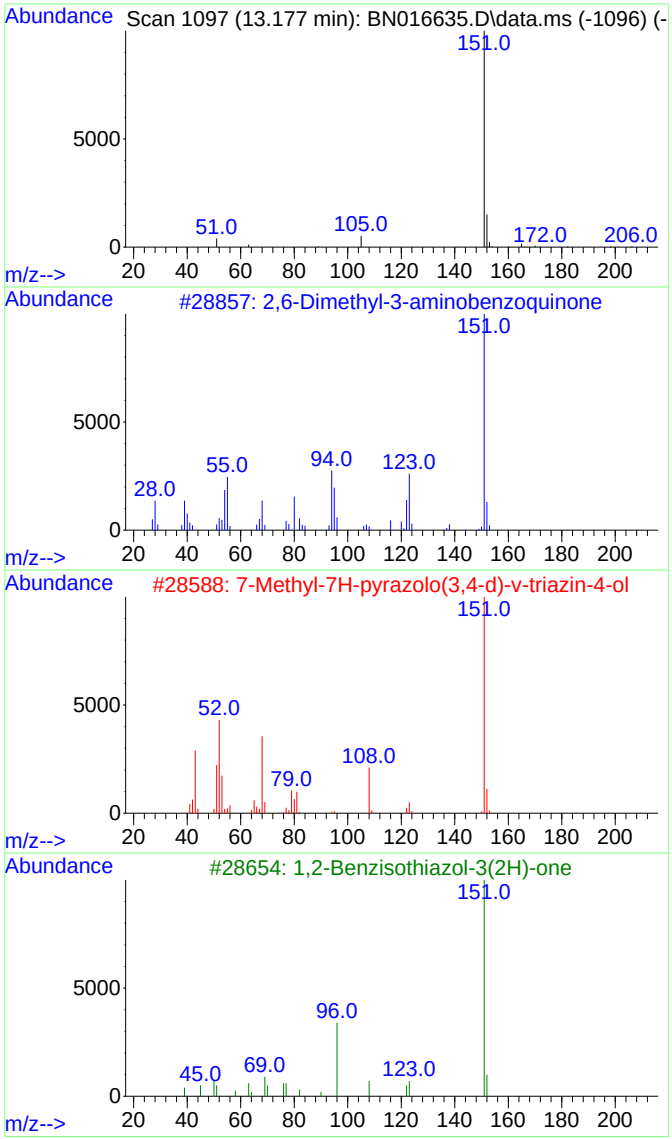
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

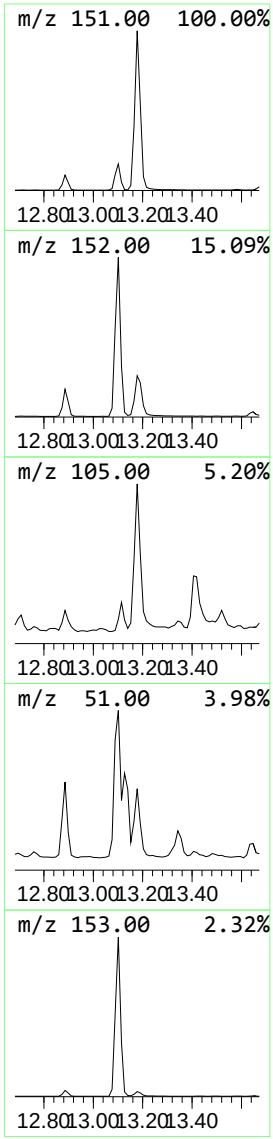
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 2,6-Dimethyl-3-aminobenzoqu... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.178	0.12 ng	55879	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6-Dimethyl-3-aminobenzoquinone	151	C8H9NO2	090005-56-4	7
2	7-Methyl-7H-pyrazolo(3,4-d)-v-tr...	151	C5H5N5O	018213-76-8	7
3	1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	7
4	Butane-1,3-dione, 1-(pyrrol-2-yl)-	151	C8H9NO2	022441-25-4	5
5	Benzoic acid, 4-(methylamino)-	151	C8H9NO2	010541-83-0	4





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ALS Vial : 4 Sample Multiplier: 1

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BNA_N
ClientSampleId :
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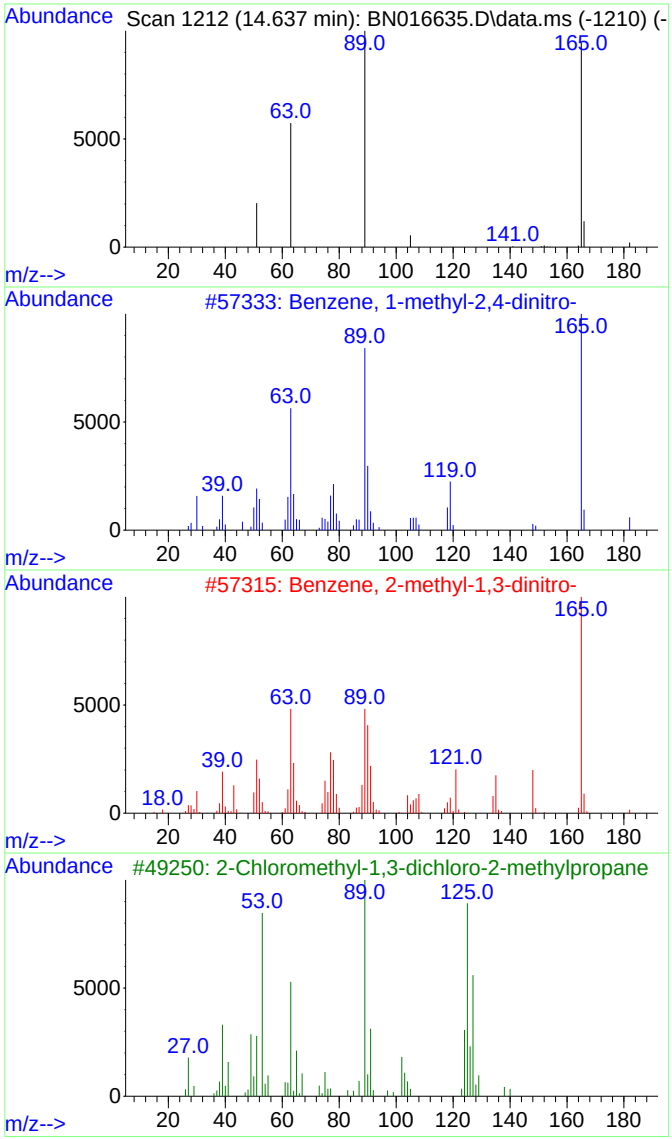
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

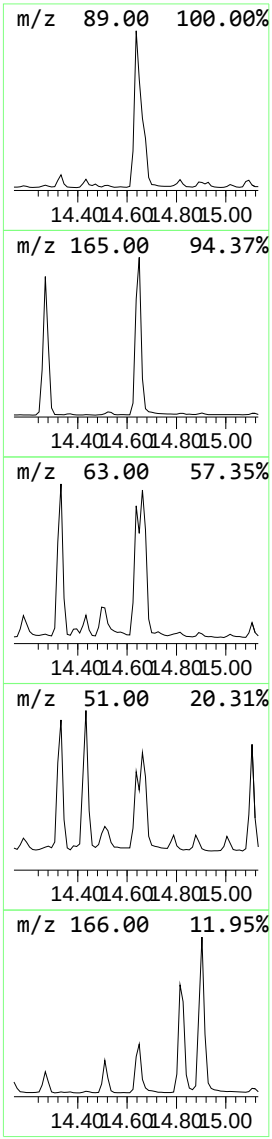
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 Benzene, 1-methyl-2,4-dinitro- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.637	0.09 ng	43283	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-2,4-dinitro-	182	C7H6N2O4	000121-14-2	74
2	Benzene, 2-methyl-1,3-dinitro-	182	C7H6N2O4	000606-20-2	38
3	2-Chloromethyl-1,3-dichloro-2-me...	174	C5H9Cl3	001067-09-0	9
4	5-[2-Chlorophenyl]tetraazole	180	C7H5ClN4	050907-46-5	9
5	6-Nitro-m-tolunitrile	162	C8H6N2O2	064113-86-6	9





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ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_N
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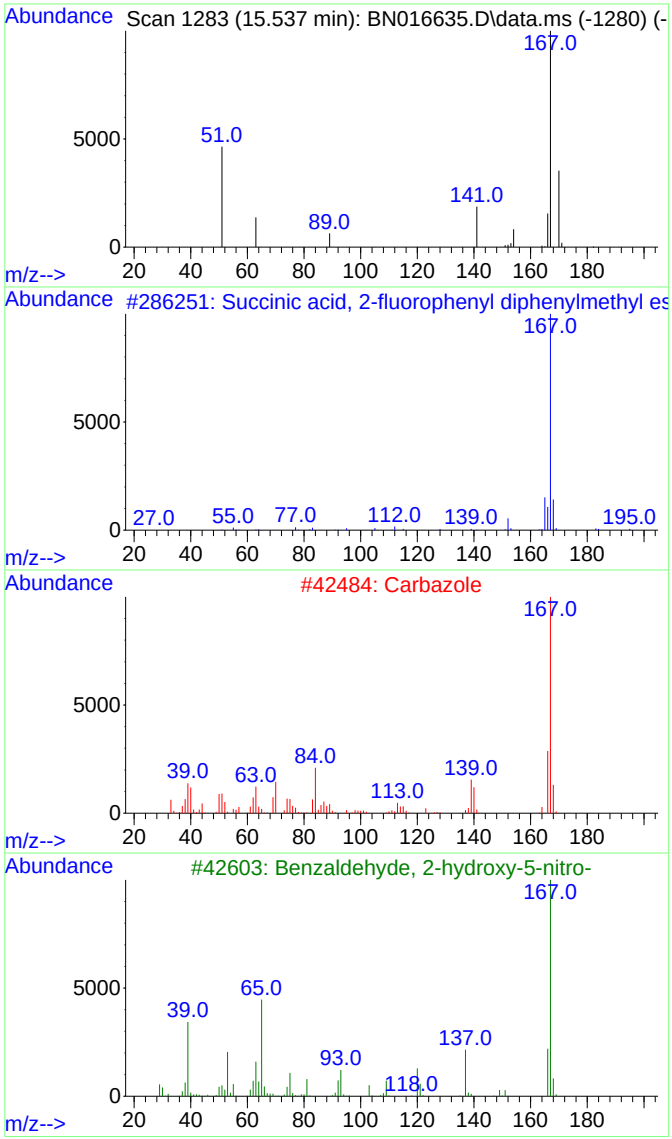
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

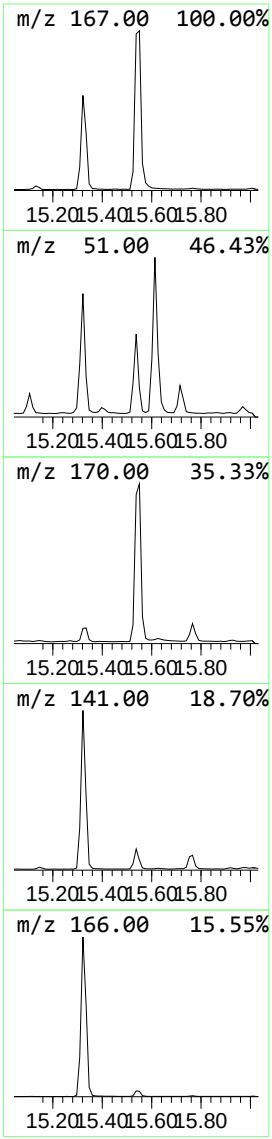
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 Succinic acid, 2-fluorophen... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.537	0.12 ng	55372	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Succinic acid, 2-fluorophenyl di...	378	C23H19FO4	1000390-17-0	9
2	Carbazole	167	C12H9N	000086-74-8	7
3	Benzaldehyde, 2-hydroxy-5-nitro-	167	C7H5NO4	000097-51-8	5
4	5-Fluoro-2-methyl-benzothiazole	167	C8H6FNS	000399-75-7	5
5	2-Azafluorene	167	C12H9N	000244-40-6	4





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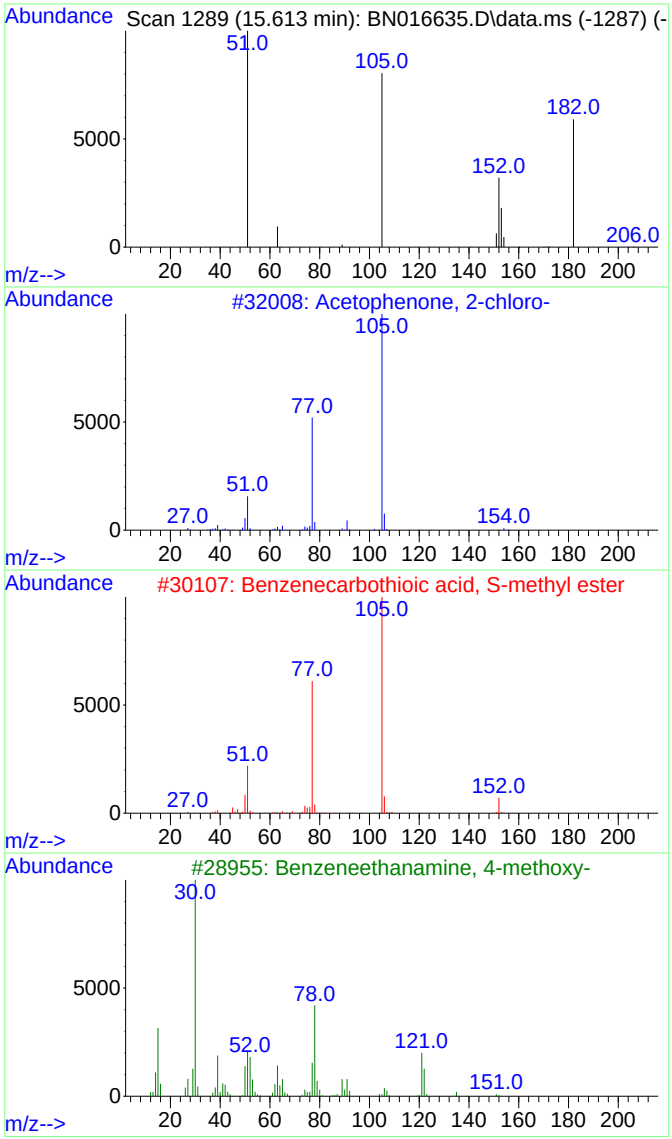
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

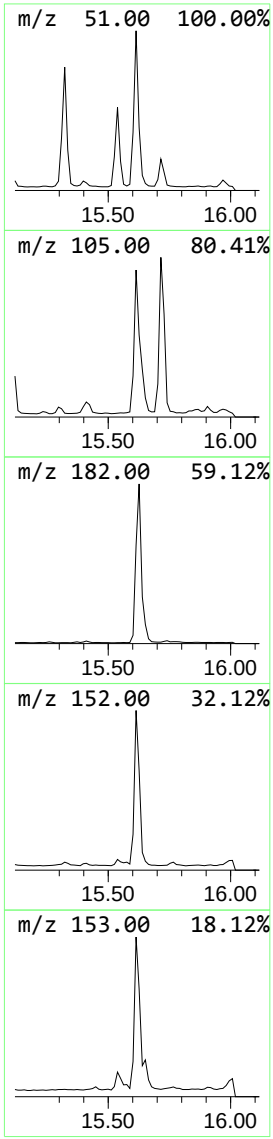
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 16 Acetophenone, 2-chloro- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.614	0.14 ng	66548	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	3
2	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	3
3	Benzeneethanamine, 4-methoxy-	151	C9H13NO	000055-81-2	3
4	Propiolonitrile	51	C3HN	001070-71-9	3
5	Propanal, 2-(benzoyloxy)-, (R)-	178	C10H10O3	078871-04-2	2





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Data File : BN016635.D
Acq On : 01 Oct 2021 14:42
Operator : CG/JU
Sample : M3990-06MS
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-836-K1-SO-1-1.5-092921MS

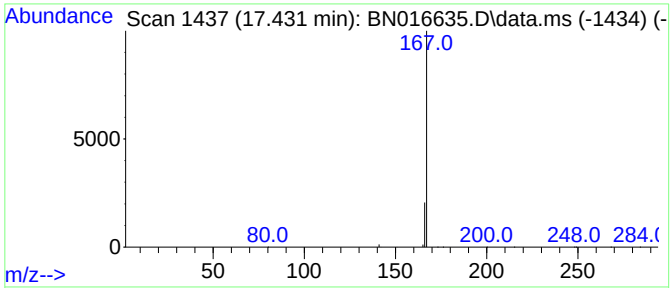
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

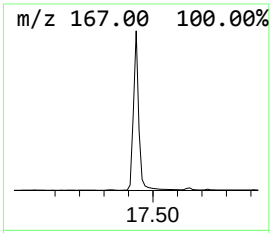
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

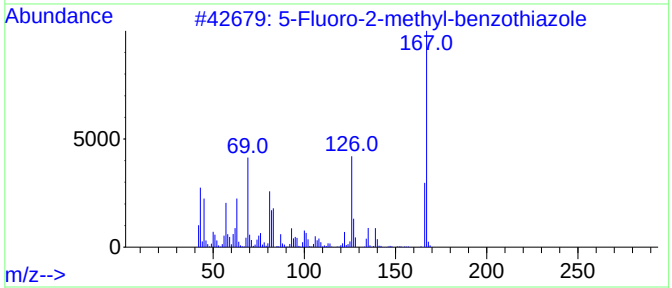
****
Peak Number 17 5-Fluoro-2-methyl-benzothia... Concentration Rank 6

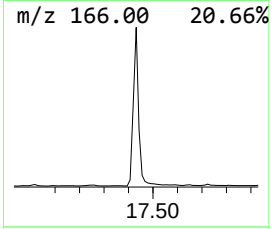
R.T.	EstConc	Area	Relative to ISTD	R.T.
17.431	0.34 ng	130622	Phenanthrene-d10	17.017

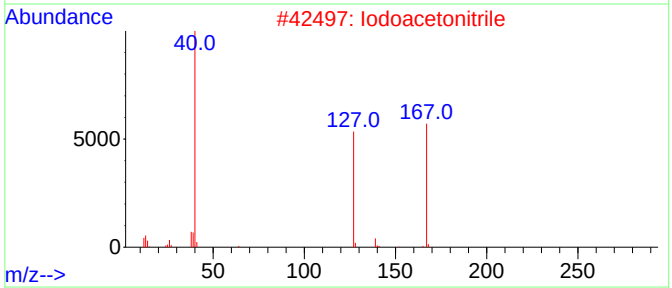
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-methyl-benzothiazole	167	C8H6FNS	000399-75-7	5
2	Iodoacetonitrile	167	C2H2IN	000624-75-9	4
3	Cycloundecene, 1-methyl-	166	C12H22	088828-82-4	4
4	1-Cyclopropanecarbonylpiperidin-...	167	C9H13NO2	063463-43-4	4
5	1,3,5-Triazine-2,4-diamine, N,N'...	167	C7H13N5	004150-59-8	4

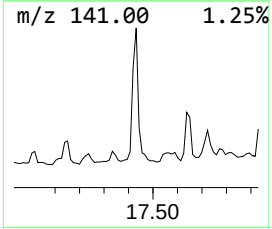


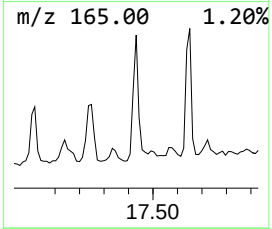


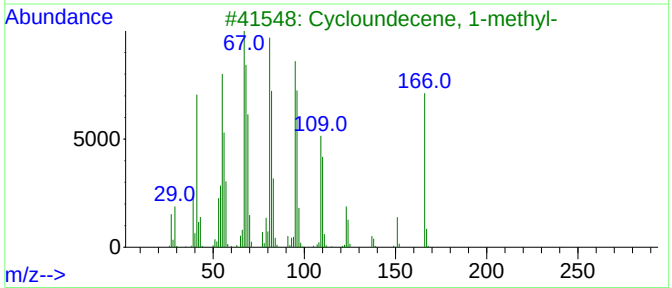


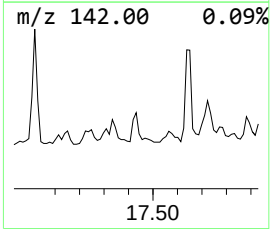












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Data File : BN016635.D
Acq On : 01 Oct 2021 14:42
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Sample : M3990-06MS
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-836-K1-SO-1-1.5-092921MS

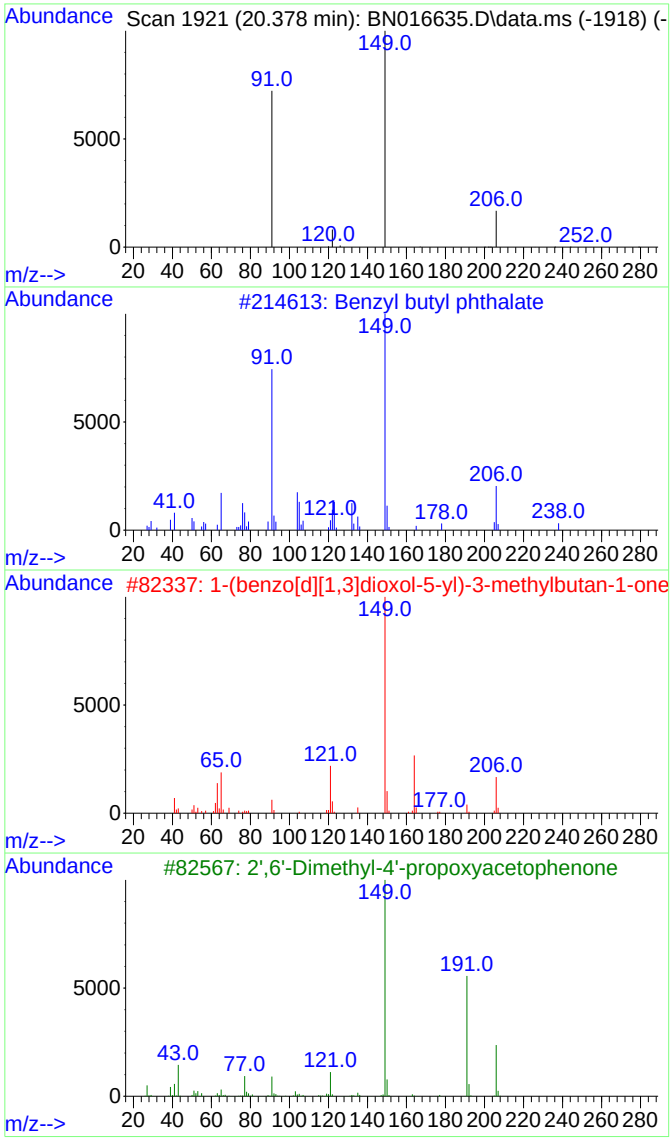
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

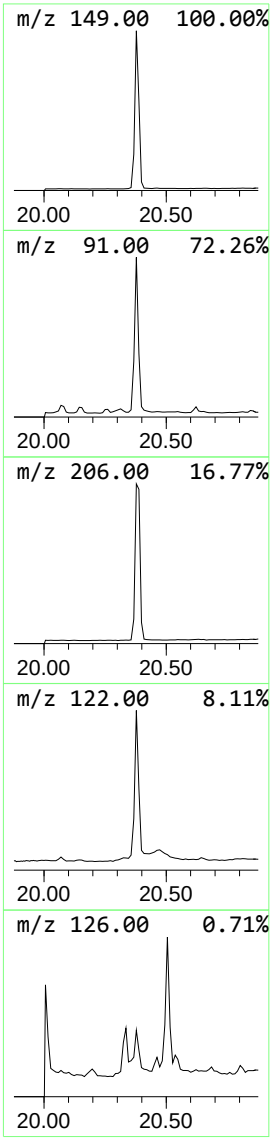
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 18 Benzyl butyl phthalate Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.378	0.10 ng	103979	Chrysene-d12	21.227

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzyl butyl phthalate	312	C19H20O4	000085-68-7	40
2	1-(benzo[d][1,3]dioxol-5-yl)-3-m...	206	C12H14O3	1000456-66-2	9
3	2',6'-Dimethyl-4'-propoxyacetoph...	206	C13H18O2	1010195-98-1	5
4	1,3,2-Dioxarsenane, 2-butyl-	206	C7H15AsO2	042541-33-3	5
5	2-tert-Butyl-6-methylphenol, n-p...	206	C14H22O	1000395-19-2	5





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ClientSampleId :
S-836-K1-SO-1-1.5-092921MS

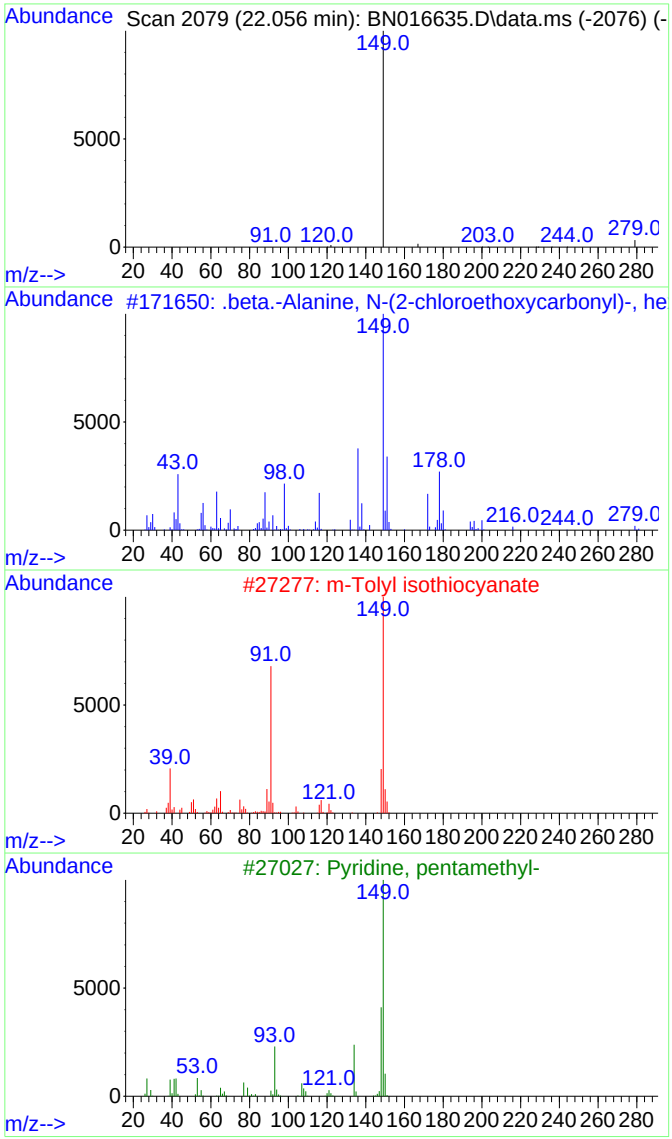
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

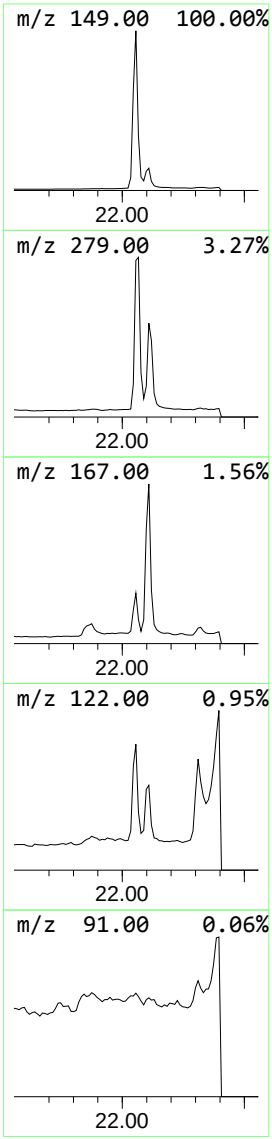
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 19 .beta.-Alanine, N-(2-chloro... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.056	0.15 ng	161053	Chrysene-d12	21.227

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Alanine, N-(2-chloroethox...	279	C12H22ClNO4	1010328-58-4	4
2	m-Tolyl isothiocyanate	149	C8H7NS	000621-30-7	4
3	Pyridine, pentamethyl-	149	C10H15N	003748-83-2	4
4	Phthalic acid, 7-bromoheptyl oct...	454	C23H35BrO4	1000415-52-2	4
5	Benzene, 1-isothiocyanato-4-methyl-	149	C8H7NS	000622-59-3	4





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Sample : M3990-06MS
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-836-K1-SO-1-1.5-092921MS

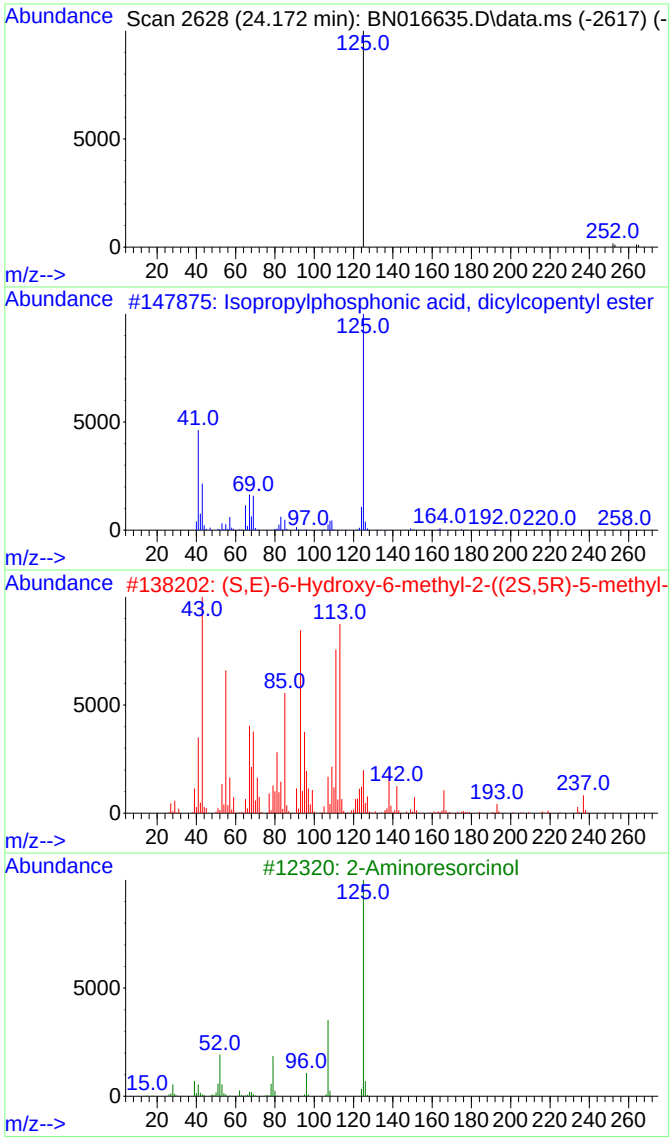
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

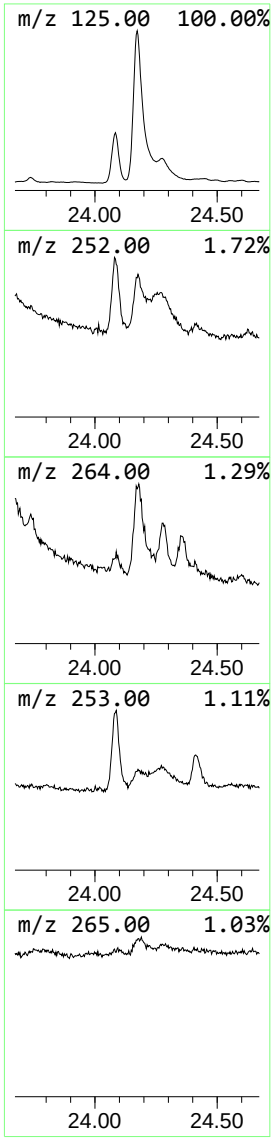
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 20 Isopropylphosphonic acid, d... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.172	0.07 ng	36812	Perylene-d12	23.481

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropylphosphonic acid, dicylc...	260	C13H25O3P	1000273-18-4	3
2	(S,E)-6-Hydroxy-6-methyl-2-((2S,...	252	C15H24O3	088243-64-5	3
3	2-Aminoresorcinol	125	C6H7NO2	003163-15-3	2
4	2-Amino-4-hydroxy-6-methylpyrimi...	125	C5H7N3O	003977-29-5	2
5	2(1H)-Pyrimidinone, 4-amino-5-me...	125	C5H7N3O	000554-01-8	2





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016635.D
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Operator : CG/JU
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Misc :
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Instrument :
BNA_N
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.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
Hydrogen isocya...	3.530	0.2	ng	50274	1	7.642	107948	0.4
1-Propanol, 2-m...	3.843	0.1	ng	38678	1	7.642	107948	0.4
Acetone	4.830	1.2	ng	317837	1	7.642	107948	0.4
1-Propanamine, ...	6.988	0.1	ng	23049	1	7.642	107948	0.4
Ethene, 1,2-dif...	7.218	0.1	ng	21185	1	7.642	107948	0.4
2-Butenal, (E)-	8.442	0.4	ng	96009	1	7.642	107948	0.4
Fomepizole	9.342	0.2	ng	76927	2	10.406	170539	0.4
5-Hydroxy-2-pyr...	9.836	0.1	ng	29042	2	10.406	170539	0.4
Propane, 1-isot...	10.204	0.9	ng	383077	2	10.406	170539	0.4
2-Propyl-4-meth...	12.301	0.4	ng	173812	2	10.406	170539	0.4
Naphthalene, 2-...	13.101	0.4	ng	181197	3	14.269	183749	0.4
Naphthalene, 2-...	13.139	0.3	ng	131196	3	14.269	183749	0.4
2,6-Dimethyl-3-...	13.178	0.1	ng	55879	3	14.269	183749	0.4
Benzene, 1-meth...	14.637	0.1	ng	43283	3	14.269	183749	0.4
Succinic acid, ...	15.537	0.1	ng	55372	3	14.269	183749	0.4
Acetophenone, 2...	15.614	0.1	ng	66548	3	14.269	183749	0.4
5-Fluoro-2-meth...	17.431	0.3	ng	130622	4	17.017	154950	0.4
Benzyl butyl ph...	20.378	0.1	ng	103979	5	21.227	417279	0.4
.beta.-Alanine,...	22.056	0.2	ng	161053	5	21.227	417279	0.4
Isopropylphosph...	24.172	0.1	ng	36812	6	23.481	197331	0.4