LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016639.D
Acq On : 01 Oct 2021 17:08
Operator : CG/JU
Sample : M4020-17
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : S-821-N-SO-2-2.5-093021

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: BN016639.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.502	44	46	59	rVB	8307	29959	4.05%	0.377%
2	4.821	185	189	197	rBV	125186	261725	35.36%	3.291%
3	5.042	210	213	220	rBV	5913	15523	2.10%	0.195%
4	5.273	234	238	250	rVB	18541	44035	5.95%	0.554%
5	6.536	371	375	381	rVB	6627	13058	1.76%	0.164%
6	6.647	383	387	391	rBV2	6341	14951	2.02%	0.188%
7	6.831	403	407	420	rVB	20486	46096	6.23%	0.580%
8	7.264	450	454	459	rVB3	5699	13920	1.88%	0.175%
9	7.643	490	495	499	rBV	50584	102039	13.79%	1.283%
10	7.864	516	519	523	rBV2	6637	13079	1.77%	0.164%
11	7.938	523	527	534	rVB	215348	384061	51.89%	4.830%
12	8.493	580	582	585	rVB	7428	12718	1.72%	0.160%
13	8.747	598	602	603	rBV2	5760	14194	1.92%	0.178%
14	8.785	603	605	610	rVB	26641	48689	6.58%	0.612%
15	10.065	703	706	712	rVB2	16939	37243	5.03%	0.468%
16	10.191	712	716	723	rBV	73473	130693	17.66%	1.644%
17	10.407	730	733	736	rBV	104073	182024	24.59%	2.289%
18	10.457	736	737	740	rVB	12924	15904	2.15%	0.200%
19	11.167	790	793	802	rBV2	7624	22766	3.08%	0.286%
20	12.003	922	931	941	rBV	43180	71026	9.60%	0.893%
21	12.078	941	948	963	rVB	10722	17167	2.32%	0.216%
22	12.301	986	998	1012	rVB	8759	14197	1.92%	0.179%
23	12.886	1071	1074	1078	rBV	74628	138966	18.78%	1.748%
24	13.178	1094	1097	1101	rBV	137035	242496	32.76%	3.049%
25	13.584	1127	1129	1132	rVB	9277	15678	2.12%	0.197%
26	13.990	1158	1161	1163	rBV	8468	13826	1.87%	0.174%
27	14.129	1168	1172	1180	rBV3	14221	35480	4.79%	0.446%
28	14.269	1180	1183	1186	rBV	140853	207501	28.03%	2.609%
29	14.345	1186	1189	1192	rVV3	23368	47167	6.37%	0.593%
30	14.523	1200	1203	1206	rVV2	35048	69566	9.40%	0.875%
31	14.599	1206	1209	1212	rVB	23885	37595	5.08%	0.473%
32	14.751	1219	1221	1223	rVV	16978	27181	3.67%	0.342%
33	14.814	1223	1226	1229	rVV2	8368	14969	2.02%	0.188%
34	15.322	1263	1266	1269	rBV2	14425	22461	3.03%	0.282%
35	15.398	1269	1272	1275	rBV3	5008	12991	1.76%	0.163%
36	15.626	1287	1290	1295	rBV3	7055	26472	3.58%	0.333%

LSC Area Percent Report

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Misc :
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Instrument : BNA_N
ClientSampleId : S-821-N-SO-2-2.5-093021

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

37	15.728	1295	1298	1300	rVV2	26492	54132	7.31%	0.681%
38	15.766	1300	1301	1304	rVV	20267	28204	3.81%	0.355%
39	15.855	1305	1308	1312	rVB2	9978	18660	2.52%	0.235%
40	16.007	1317	1320	1322	rVB	161288	179481	24.25%	2.257%
41	16.336	1341	1347	1349	rBV5	3882	14189	1.92%	0.178%
42	16.592	1365	1368	1370	rBV	7791	13182	1.78%	0.166%
43	16.847	1386	1389	1394	rVB2	7013	16324	2.21%	0.205%
44	17.018	1397	1403	1405	rBV	107125	192024	25.94%	2.415%
45	17.066	1405	1407	1410	rVV	70158	101560	13.72%	1.277%
46	17.152	1411	1414	1417	rVB	15237	25473	3.44%	0.320%
47	17.225	1417	1420	1425	rBV	21303	48543	6.56%	0.610%
48	17.310	1425	1427	1431	rVV3	5461	12711	1.72%	0.160%
49	17.431	1435	1437	1442	rBV2	6034	13531	1.83%	0.170%
50	17.784	1463	1466	1474	rVV	42451	98276	13.28%	1.236%
51	17.918	1474	1477	1478	rVV	21538	41519	5.61%	0.522%
52	17.955	1478	1480	1483	rVV	28360	62814	8.49%	0.790%
53	18.003	1483	1484	1486	rVB	20454	12077	1.63%	0.152%
54	18.909	1661	1665	1674	rVB	14841	19880	2.69%	0.250%
55	19.063	1689	1696	1699	rBV	100722	143689	19.41%	1.807%
56	19.098	1699	1703	1712	rVV	129701	179118	24.20%	2.252%
57	19.177	1715	1719	1728	rVV2	8992	20025	2.71%	0.252%
58	19.242	1728	1732	1747	rVB2	10107	18319	2.48%	0.230%
59	19.460	1767	1776	1788	rVB	125777	176911	23.90%	2.225%
60	19.599	1799	1804	1808	rBV	29277	35852	4.84%	0.451%
61	19.644	1808	1813	1815	rVV2	13899	20019	2.70%	0.252%
62	19.679	1815	1820	1823	rVV	86731	106578	14.40%	1.340%
63	19.708	1823	1826	1836	rVV	32481	44525	6.02%	0.560%
64	19.783	1836	1841	1846	rVV	23036	31202	4.22%	0.392%
65	20.006	1884	1886	1888	rBV2	30811	34782	4.70%	0.437%
66	20.059	1888	1891	1894	rVV2	13605	39293	5.31%	0.494%
67	20.112	1894	1896	1897	rBV	11222	15165	2.05%	0.191%
68	20.335	1914	1917	1920	rVB	31696	42237	5.71%	0.531%
69	20.537	1933	1936	1941	rVB2	43580	64502	8.71%	0.811%
70	20.643	1944	1946	1949	rVB	17869	24447	3.30%	0.307%
71	20.718	1950	1953	1957	rBV2	17207	33435	4.52%	0.420%
72	20.877	1966	1968	1970	rVB2	18658	24548	3.32%	0.309%
73	20.973	1970	1977	1980	rBV3	100793	195740	26.45%	2.461%
74	21.026	1980	1982	1986	rVB	14058	21553	2.91%	0.271%
75	21.164	1993	1995	1997	rBV	51580	67795	9.16%	0.853%
76	21.228	1997	2001	2004	rVV2	171901	343179	46.37%	4.316%

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

77	21.270	2004	2005	2010	rVV	61479	62223	8.41%	0.782%
78	21.334	2010	2011	2015	rVB3	11219	16679	2.25%	0.210%
79	21.599	2033	2036	2039	rBV3	9094	15681	2.12%	0.197%
80	21.748	2047	2050	2056	rVB3	16066	32916	4.45%	0.414%
81	21.875	2056	2062	2067	rVV2	94556	253314	34.22%	3.186%
82	22.003	2071	2074	2078	rVV	125479	192378	25.99%	2.419%
83	22.109	2081	2084	2089	rVB2	52631	75392	10.19%	0.948%
84	22.321	2097	2104	2110	rBV2	94515	277325	37.47%	3.487%
85	22.554	2150	2155	2171	rVB2	18732	28049	3.79%	0.353%
86	22.807	2220	2229	2234	rBV	46511	84892	11.47%	1.068%
87	22.892	2247	2254	2271	rVB	97523	165822	22.40%	2.085%
88	22.978	2272	2279	2307	rVB2	23537	48035	6.49%	0.604%
89	23.289	2361	2370	2381	rVB2	28426	51829	7.00%	0.652%
90	23.385	2389	2398	2406	rBV	34464	64051	8.65%	0.805%
91	23.485	2416	2427	2432	rBV	127337	229613	31.02%	2.887%
92	23.533	2433	2441	2482	rVB	382927	740154	100.00%	9.308%
93	23.741	2496	2502	2514	rVB	11900	20015	2.70%	0.252%
94	24.090	2594	2604	2616	rVB	27464	57038	7.71%	0.717%
95	24.176	2618	2629	2652	rBV	101836	243366	32.88%	3.060%
96	25.764	3079	3093	3119	rVB2	26822	79160	10.70%	0.995%
97	25.915	3125	3137	3162	rVB	11699	36833	4.98%	0.463%
98	26.462	3281	3297	3328	rVB	18838	61742	8.34%	0.776%
99	26.630	3335	3346	3360	rBV	5856	17785	2.40%	0.224%
100	27.493	3585	3598	3644	rVB2	10648	44864	6.06%	0.564%

Sum of corrected areas: 7952066

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Data File : BN016639.D
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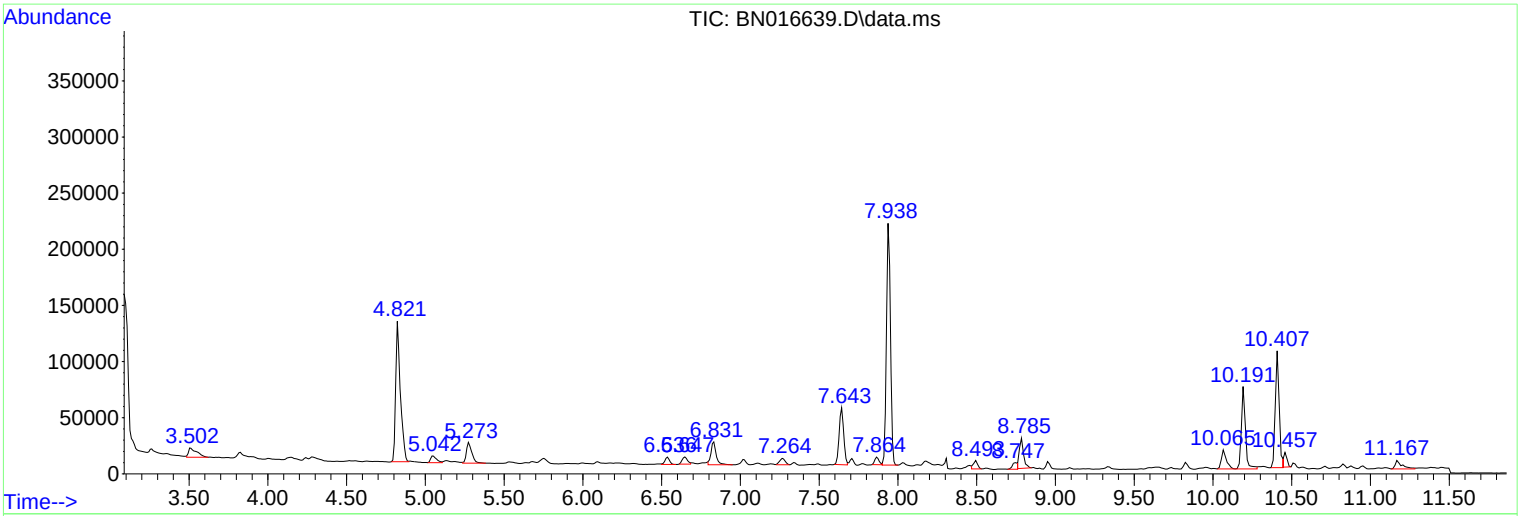
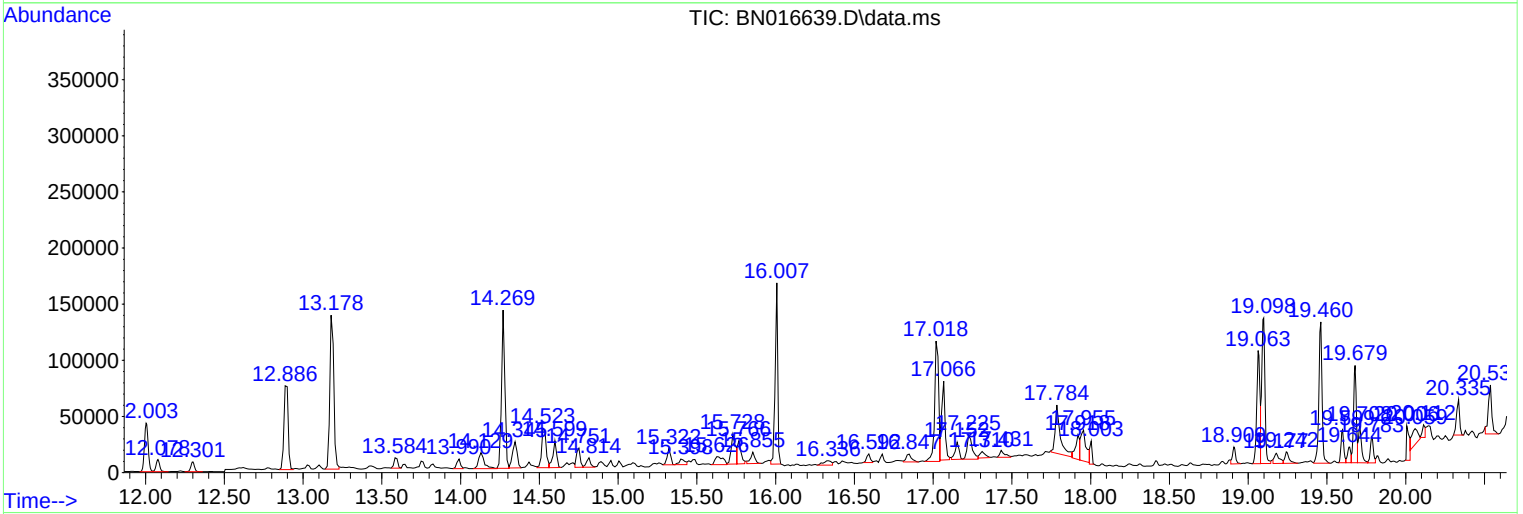
Misc :
ALS Vial : 8 Sample Multiplier: 1

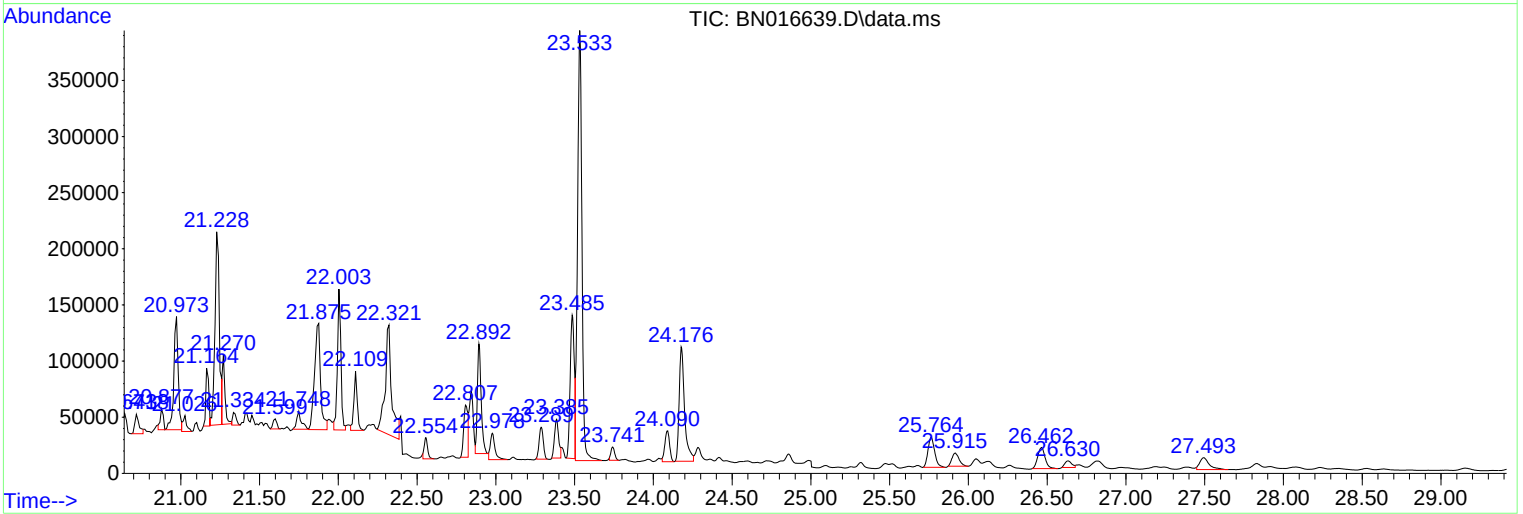
Instrument :
BNA_N
ClientSampleId :
S-821-N-SO-2-2.5-093021

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







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Instrument :
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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

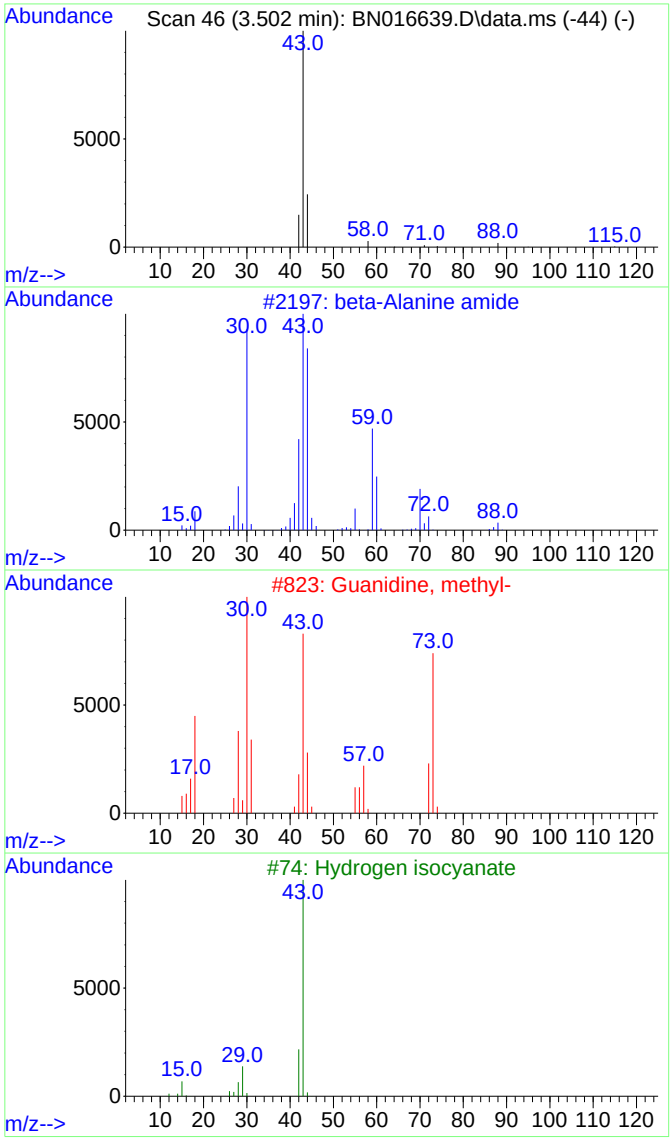
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

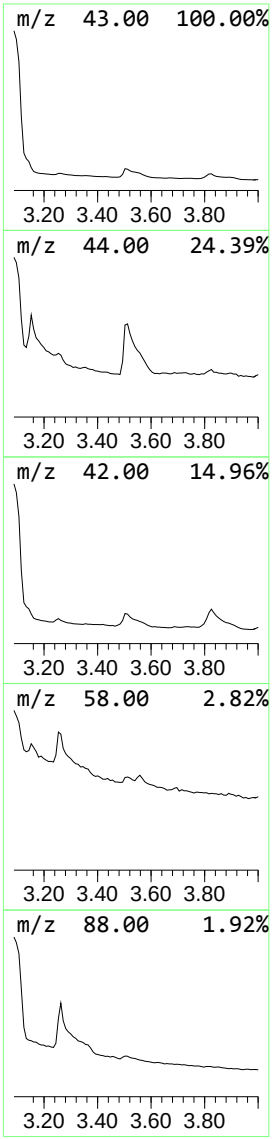
****

Peak Number 1 beta-Alanine amide Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.502	0.12 ng	29959	1,4-Dichlorobenzene-d4	7.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	beta-Alanine amide	88	C3H8N2O	004726-85-6	7
2	Guanidine, methyl-	73	C2H7N3	000471-29-4	4
3	Hydrogen isocyanate	43	CHNO	000075-13-8	3
4	Hydrogen azide	43	HN3	007782-79-8	3
5	Isobutane	58	C4H10	000075-28-5	3





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S-821-N-SO-2-2.5-093021

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

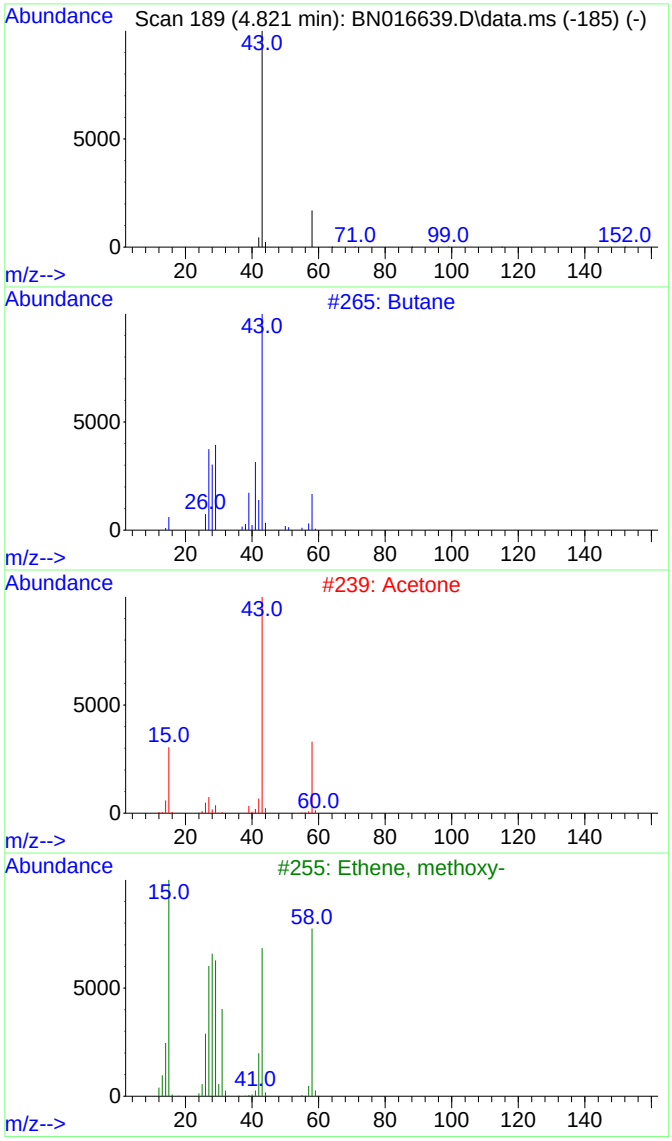
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

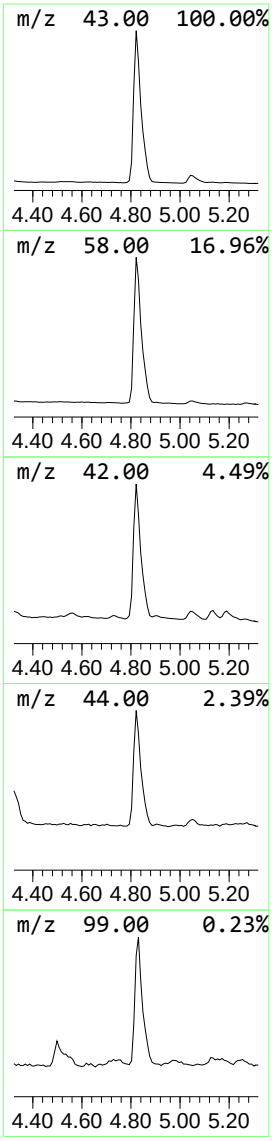
****

Peak Number 2 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	1.03 ng	261725	1,4-Dichlorobenzene-d4	7.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	4
2	Acetone	58	C3H6O	000067-64-1	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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Sample : M4020-17
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : S-821-N-SO-2-2.5-093021

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

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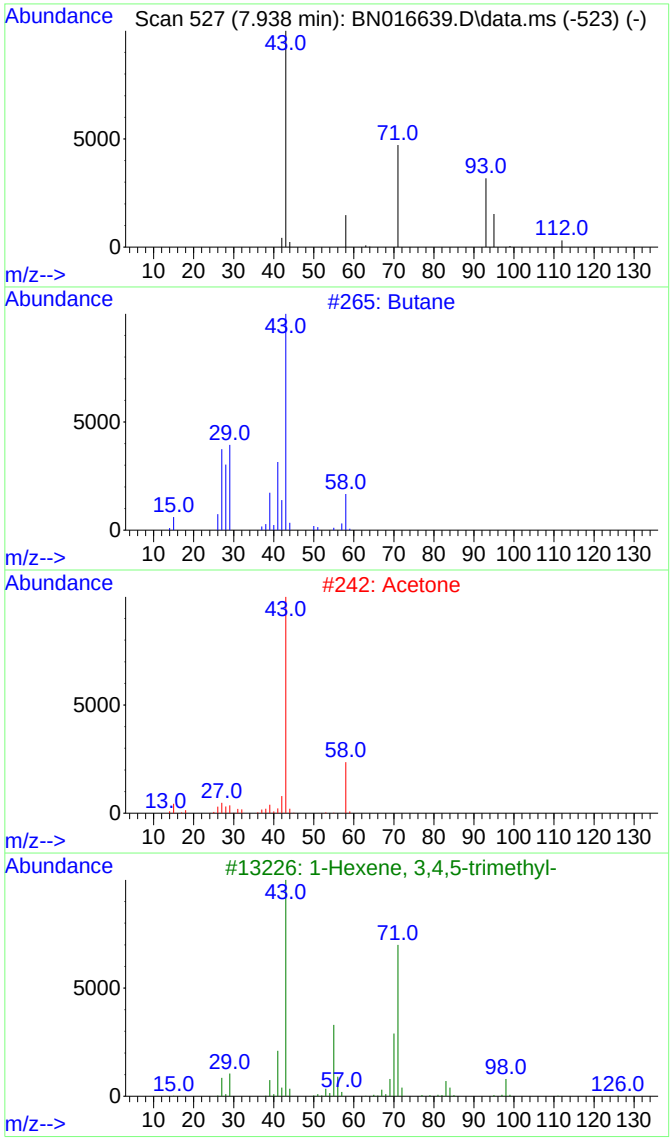
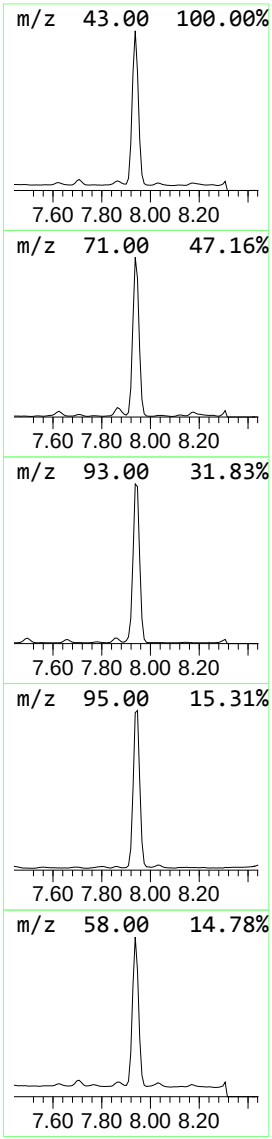
Peak Number 3 Butane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.938	1.51 ng	384061	1,4-Dichlorobenzene-d4	7.643

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	4
2	Acetone	58	C3H6O	000067-64-1	4
3	1-Hexene, 3,4,5-trimethyl-	126	C9H18	056728-10-0	4
4	2-Propenamide	71	C3H5NO	000079-06-1	3
5	Cyanic acid, ethyl ester	71	C3H5NO	000627-48-5	3





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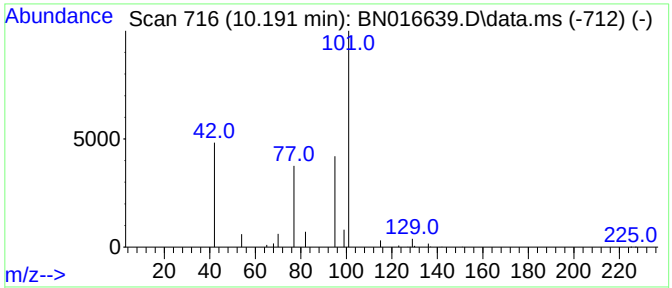
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

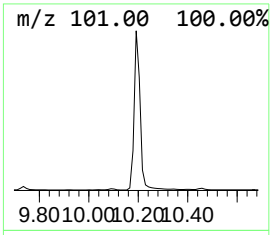
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

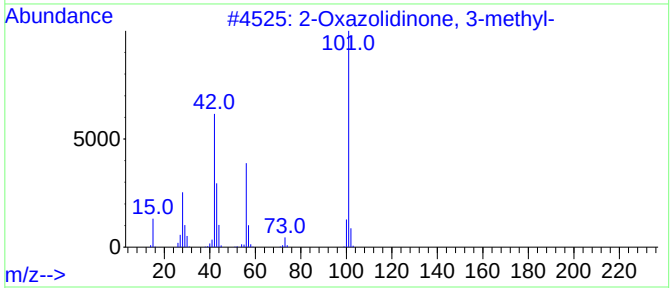
****
Peak Number 4 2-Oxazolidinone, 3-methyl- Concentration Rank 8

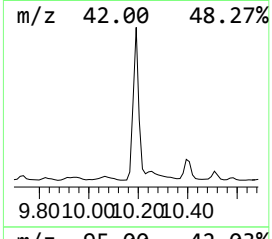
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.191	0.29 ng	130693	Naphthalene-d8	10.407

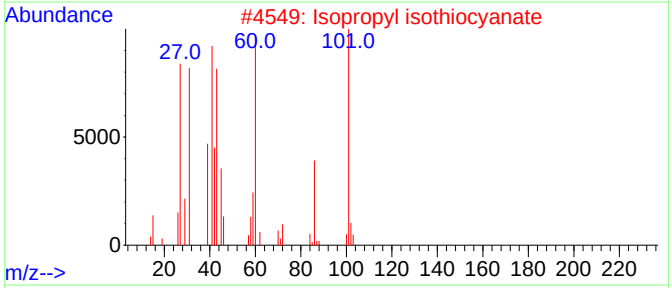
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Oxazolidinone, 3-methyl-	101	C4H7NO2	019836-78-3	5
2	Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	5
3	3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	5
4	Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	5
5	3-Aminopropionitrile	70	C3H6N2	000151-18-8	4

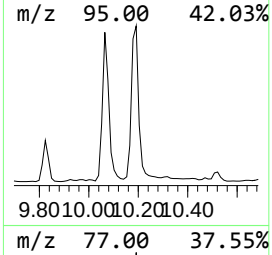


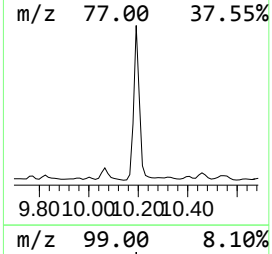


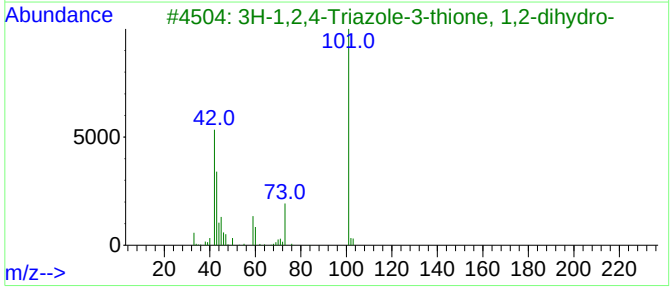


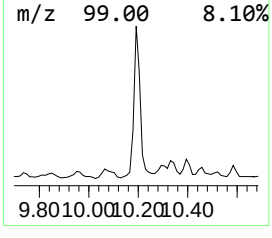












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Acq On : 01 Oct 2021 17:08
Operator : CG/JU
Sample : M4020-17
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : S-821-N-SO-2-2.5-093021

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

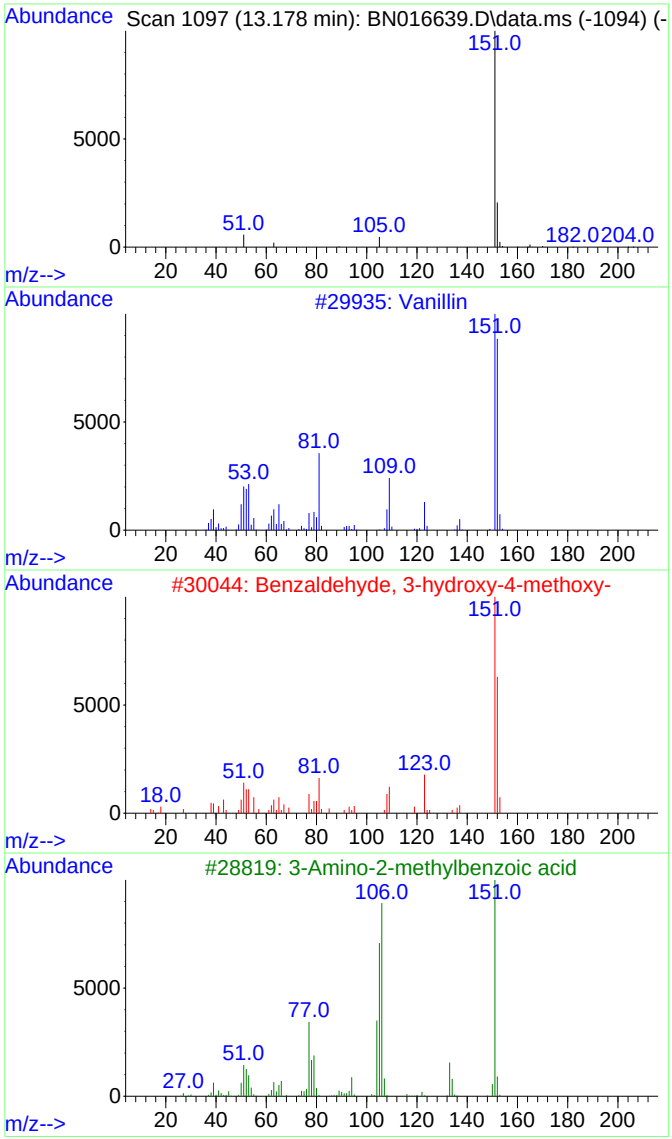
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

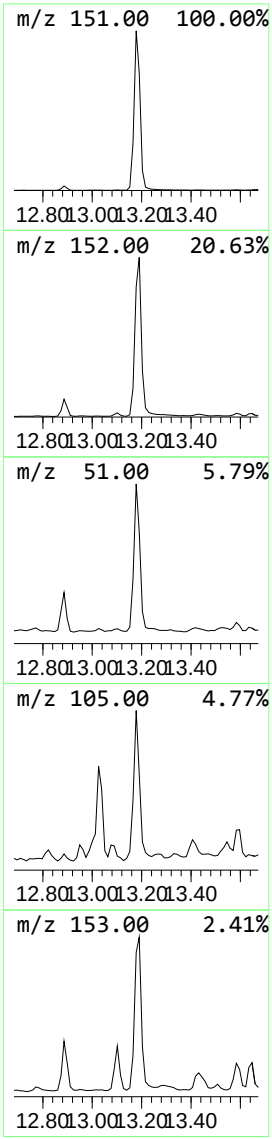
****

Peak Number 5 Vanillin Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.178	0.47 ng	242496	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Vanillin	152	C8H8O3	000121-33-5	5
2	Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	4
3	3-Amino-2-methylbenzoic acid	151	C8H9NO2	052130-17-3	4
4	1,2,4-Triazolo[4,3-a]pyridine-3(...	151	C6H5N3S	006952-68-7	4
5	Thiazolo[5,4-d]pyrimidine, 7-met...	151	C6H5N3S	013316-06-8	4





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Operator : CG/JU
Sample : M4020-17
Misc :
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Instrument :
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ClientSampleId :
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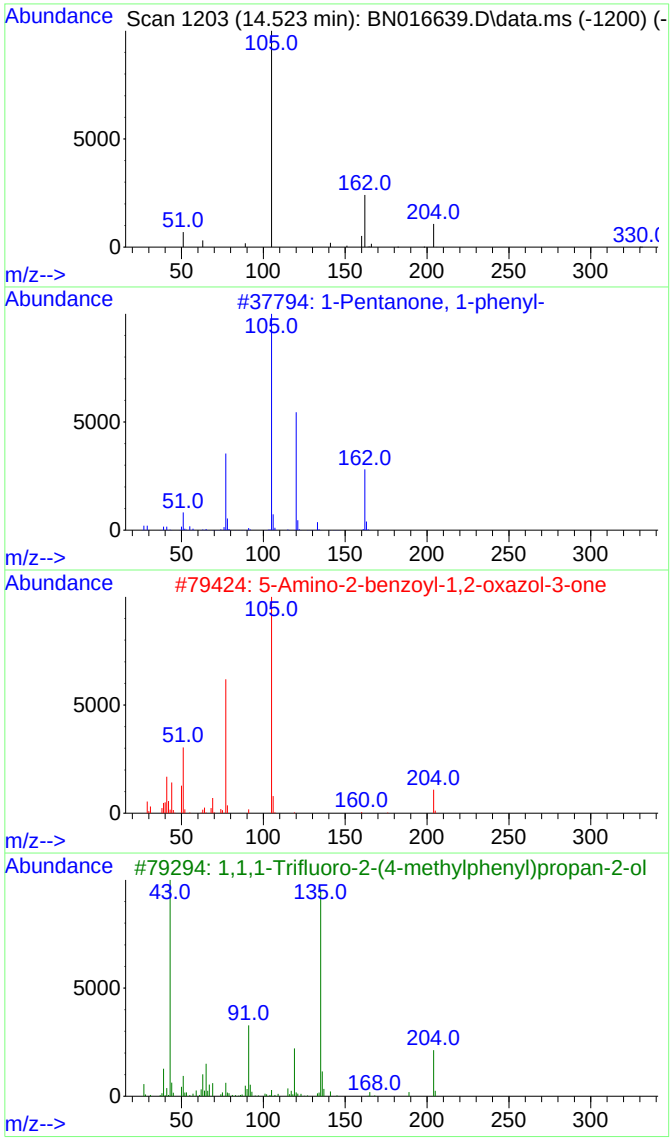
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

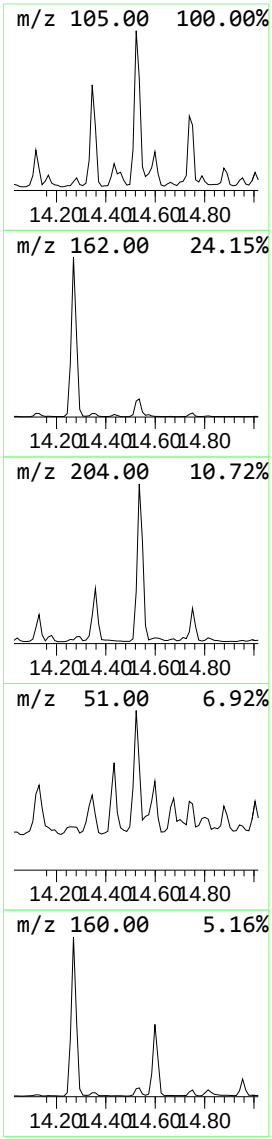
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1-Pentanone, 1-phenyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.523	0.13 ng	69566	Acenaphthene-d10	14.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentanone, 1-phenyl-	162	C11H14O	001009-14-9	5
2	5-Amino-2-benzoyl-1,2-oxazol-3-one	204	C10H8N2O3	090771-25-8	5
3	1,1,1-Trifluoro-2-(4-methylpheny...	204	C10H11F3O	076953-97-4	5
4	2-Propenoic acid, 2-bromo-, meth...	164	C4H5BrO2	004519-46-4	4
5	Benzene, 1-methyl-2-(1-ethylprop...	162	C12H18	054410-74-1	4





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Misc :
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Instrument :
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ClientSampleId :
S-821-N-SO-2-2.5-093021

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

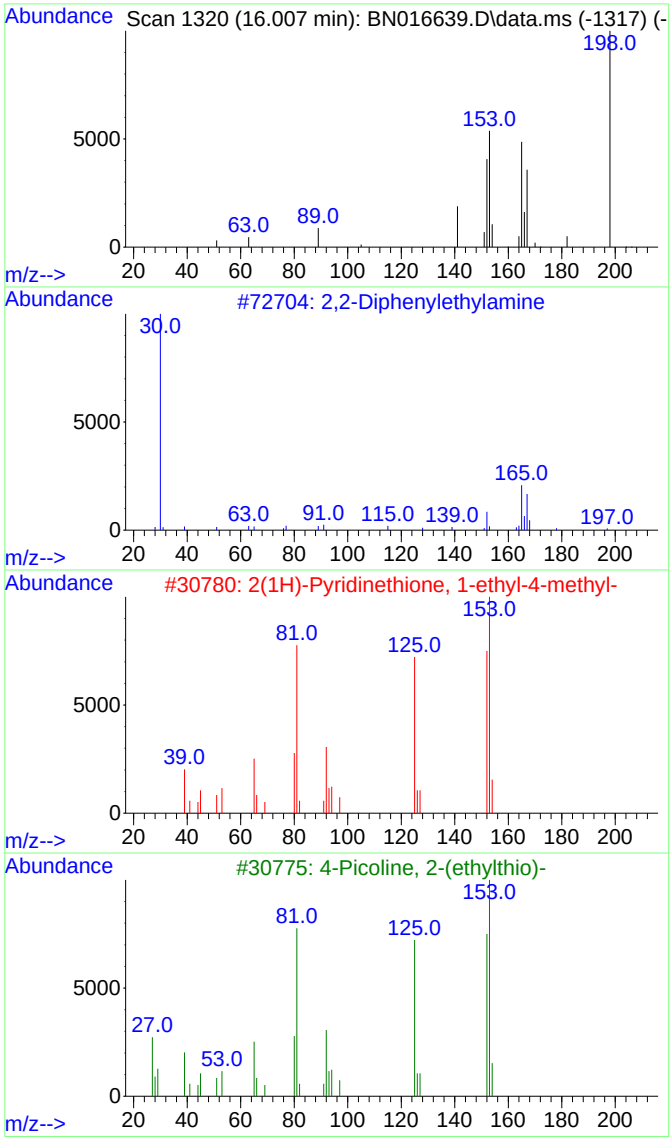
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

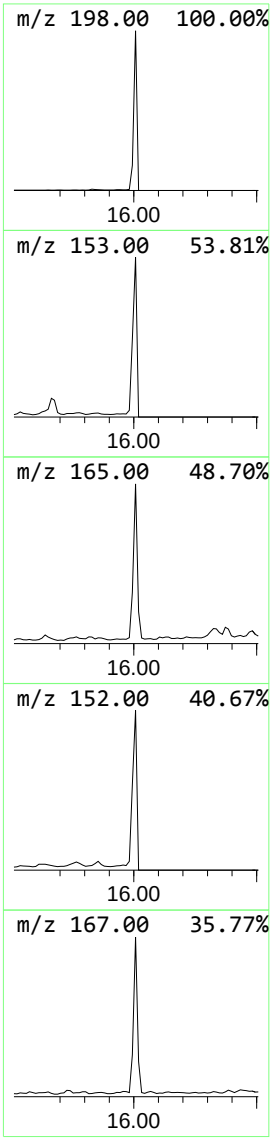
****

Peak Number 7 2,2-Diphenylethylamine Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.007	0.37 ng	179481	Phenanthrene-d10	17.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2-Diphenylethylamine	197	C14H15N	003963-62-0	12
2	2(1H)-Pyridinethione, 1-ethyl-4-...	153	C8H11NS	019006-72-5	9
3	4-Picoline, 2-(ethylthio)-	153	C8H11NS	019006-78-1	9
4	2(1H)-Pyridinethione, 1-ethyl-6-...	153	C8H11NS	019006-73-6	9
5	2,4-Dimethyl-6-(methylthio)pyridine	153	C8H11NS	1000305-54-7	9





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Misc :
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S-821-N-SO-2-2.5-093021

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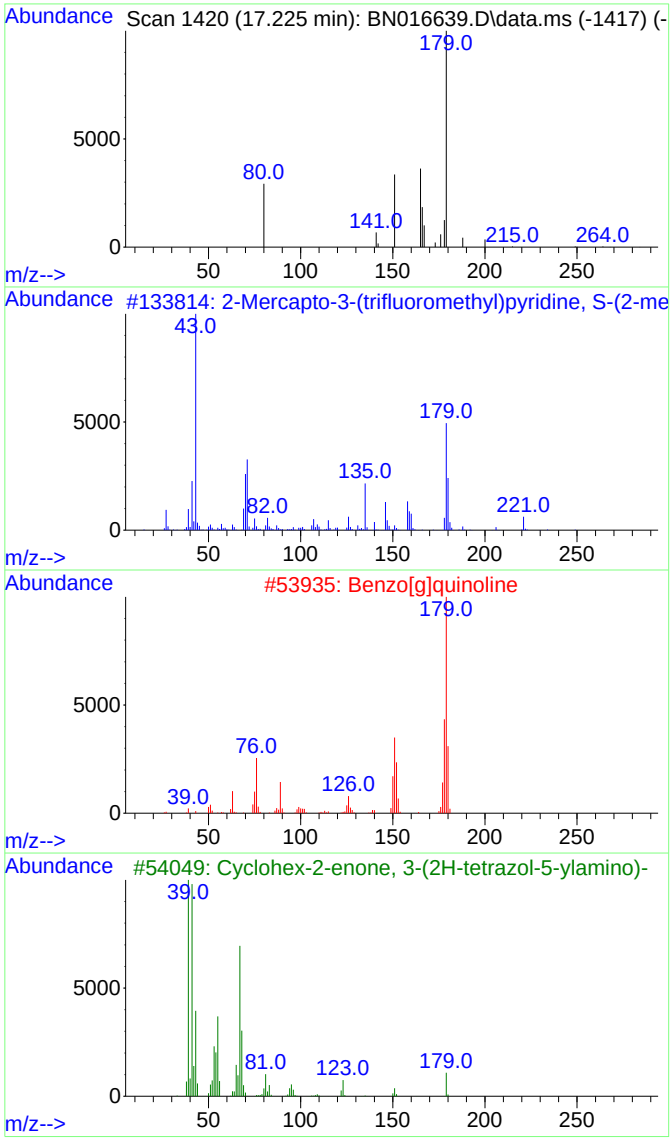
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

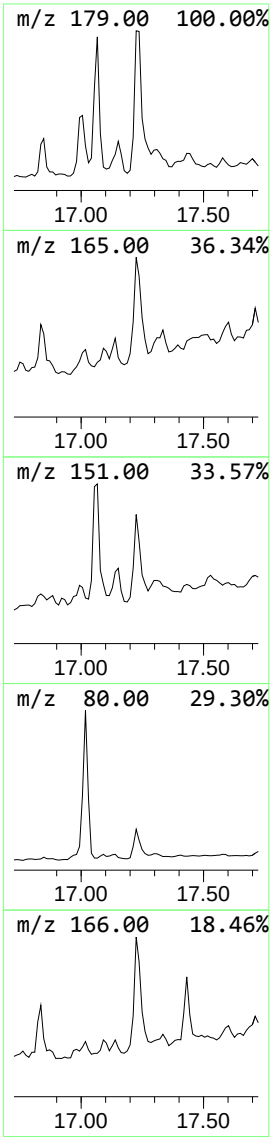
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 2-Mercapto-3-(trifluorometh... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.225	0.10 ng	48543	Phenanthrene-d10	17.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Mercapto-3-(trifluoromethyl)py...	249	C10H10F3NOS	1000463-17-8	7
2	Benzo[g]quinoline	179	C13H9N	000260-36-6	7
3	Cyclohex-2-enone, 3-(2H-tetrazol...	179	C7H9N5O	1000311-07-7	5
4	Benzo[f]quinoline	179	C13H9N	000085-02-9	5
5	Ethyl N-(o-anisyl)formimidate	179	C10H13NO2	015296-48-7	5





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Sample : M4020-17
Misc :
ALS Vial : 8 Sample Multiplier: 1

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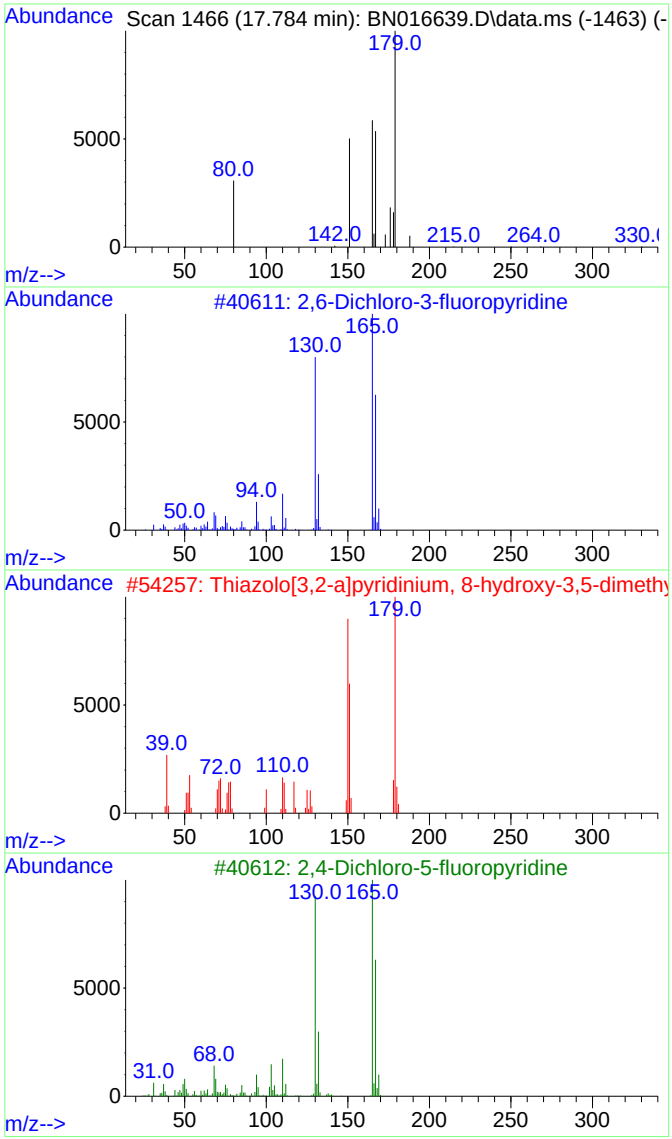
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

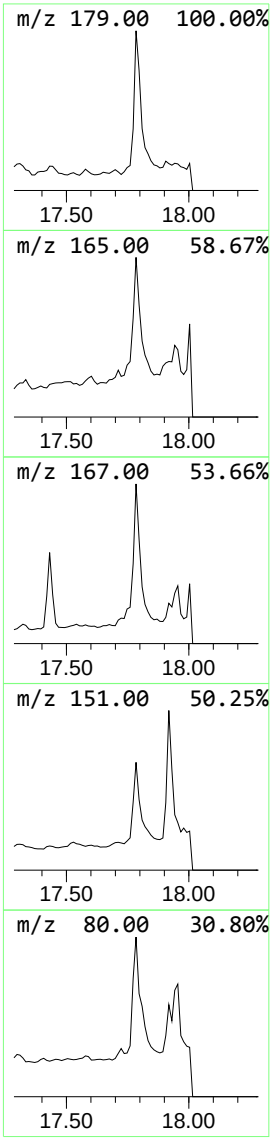
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 2,6-Dichloro-3-fluoropyridine Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.784	0.20 ng	98276	Phenanthrene-d10	17.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6-Dichloro-3-fluoropyridine	165	C5H2Cl2FN	052208-50-1	9
2	Thiazolo[3,2-a]pyridinium, 8-hyd...	179	C9H9NOS	030277-00-0	9
3	2,4-Dichloro-5-fluoropyridine	165	C5H2Cl2FN	189281-48-9	9
4	s-Triazolo[4,3-a]pyridine-3-thio...	165	C7H7N3S	004926-22-1	7
5	3-Methoxy-1-methyl-1H-pirazolo[4...	165	C6H7N5O	037526-55-9	7





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Misc :
ALS Vial : 8 Sample Multiplier: 1

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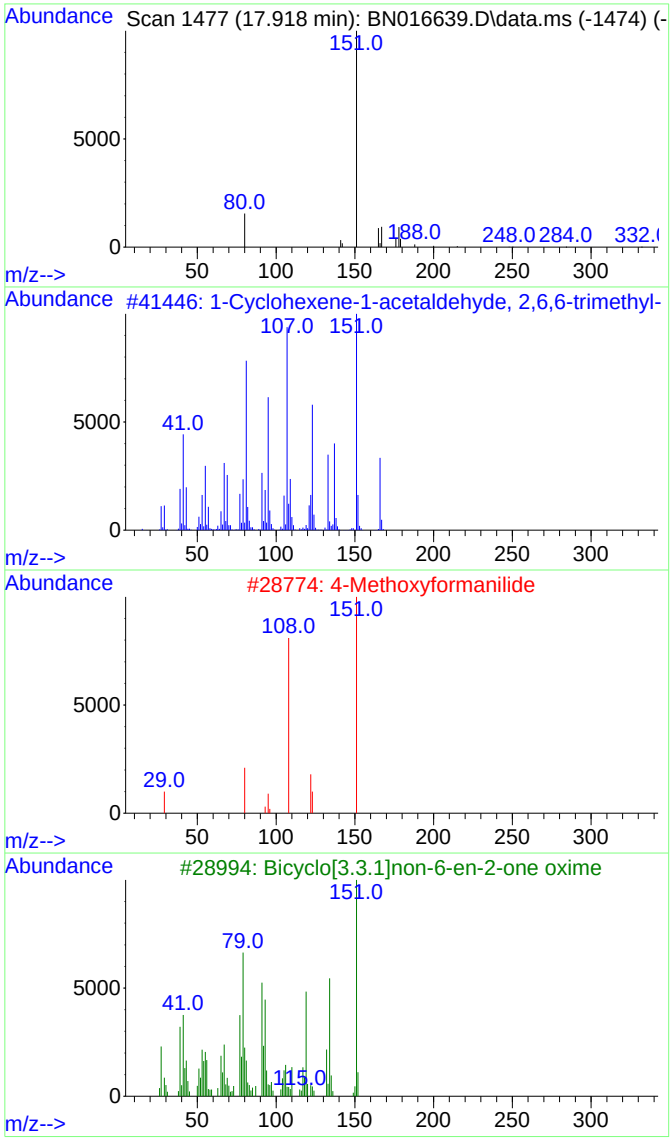
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

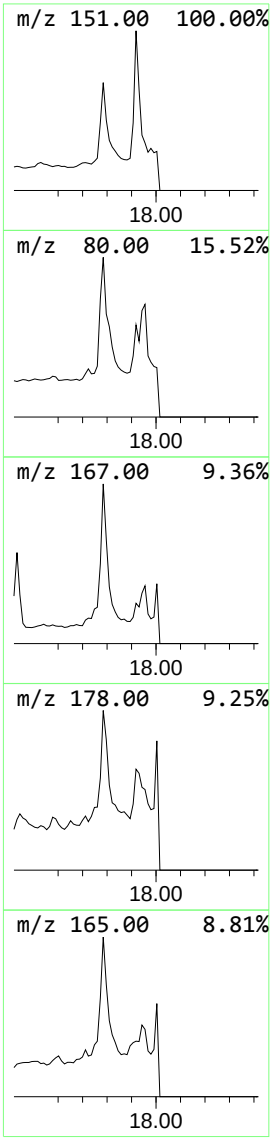
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1-Cyclohexene-1-acetaldehyd... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.918	0.09 ng	41519	Phenanthrene-d10	17.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Cyclohexene-1-acetaldehyde, 2,...	166	C11H18O	000472-66-2	5
2	4-Methoxyformanilide	151	C8H9NO2	005470-34-8	5
3	Bicyclo[3.3.1]non-6-en-2-one oxime	151	C9H13NO	1000186-04-7	5
4	5-Deoxypyridoxal	151	C8H9NO2	001849-49-6	4
5	Benzofuran-4(5H)-one, 6,7-dihydr...	151	C8H9NO2	061190-46-3	4





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Operator : CG/JU
Sample : M4020-17
Misc :
ALS Vial : 8 Sample Multiplier: 1

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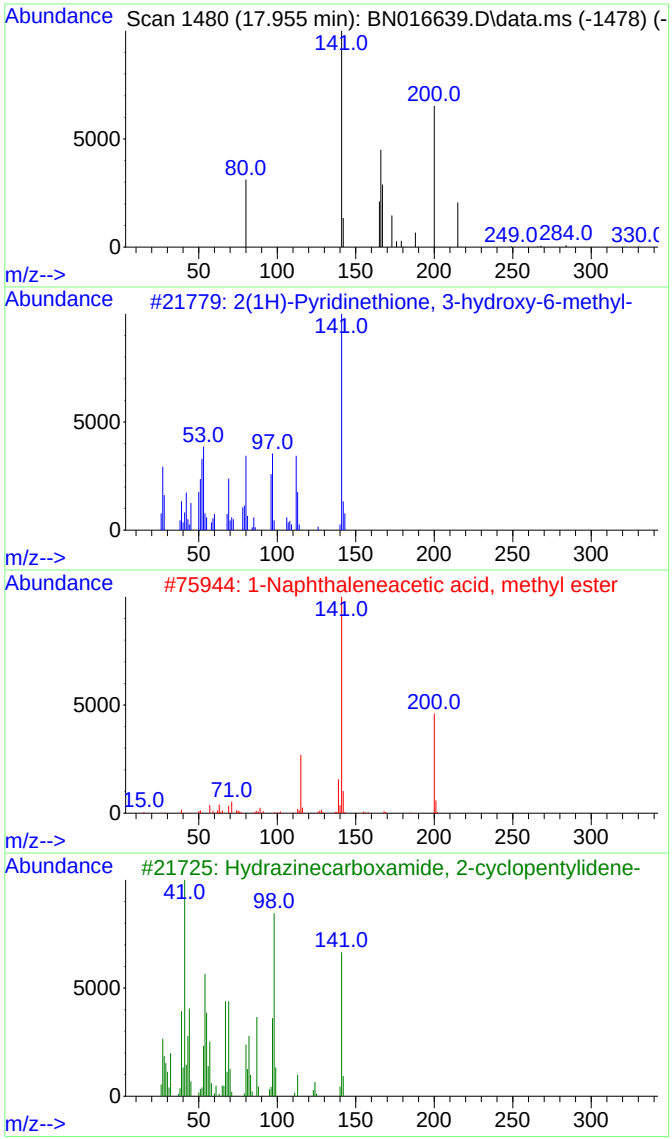
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

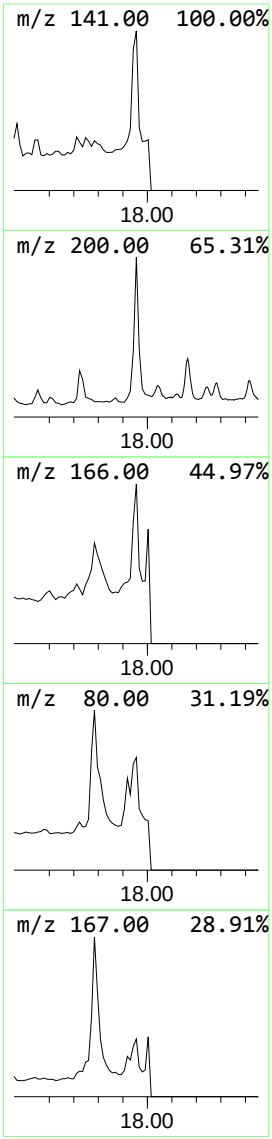
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 2(1H)-Pyridinethione, 3-hyd... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.955	0.13 ng	62814	Phenanthrene-d10	17.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)-Pyridinethione, 3-hydroxy-...	141	C6H7NOS	022989-67-9	9
2	1-Naphthaleneacetic acid, methyl...	200	C13H12O2	002876-78-0	9
3	Hydrazinecarboxamide, 2-cyclopen...	141	C6H11N3O	005459-00-7	9
4	4-Chlorophenoxyacetic acid, meth...	200	C9H9ClO3	1000362-94-5	9
5	Atrazine	215	C8H14ClN5	001912-24-9	9





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Sample : M4020-17
Misc :
ALS Vial : 8 Sample Multiplier: 1

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S-821-N-SO-2-2.5-093021

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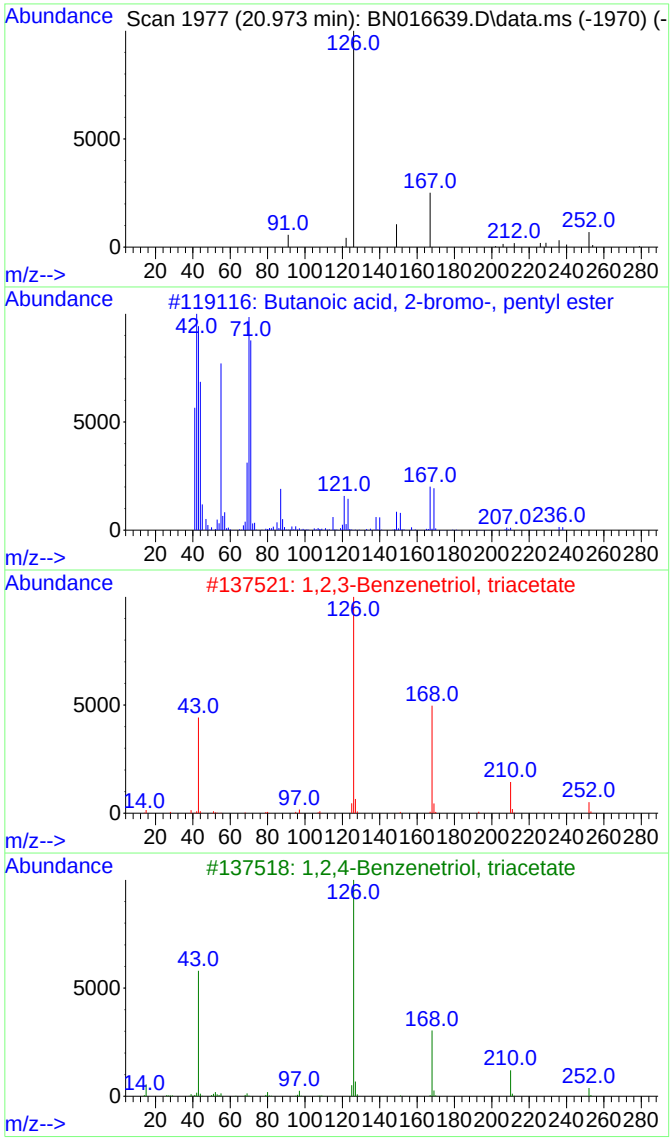
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

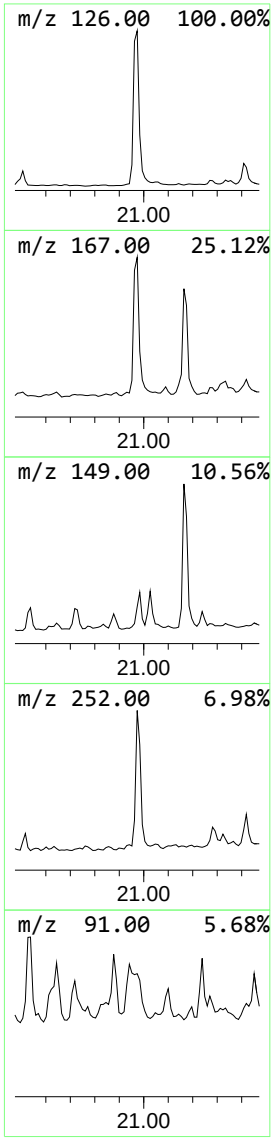
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 Butanoic acid, 2-bromo-, pe... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.973	0.23 ng	195740	Chrysene-d12	21.227

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 2-bromo-, pentyl ...	236	C9H17BrO2	1000131-81-8	5
2	1,2,3-Benzenetriol, triacetate	252	C12H12O6	000525-52-0	4
3	1,2,4-Benzenetriol, triacetate	252	C12H12O6	000613-03-6	4
4	(6S,12aR,E)-2,2-Dimethyltetrahyd...	236	C14H24N2O	155975-43-2	4
5	N-[[6-Cyclooctylaminohexyl]aziri...	252	C16H32N2	1010256-12-1	4





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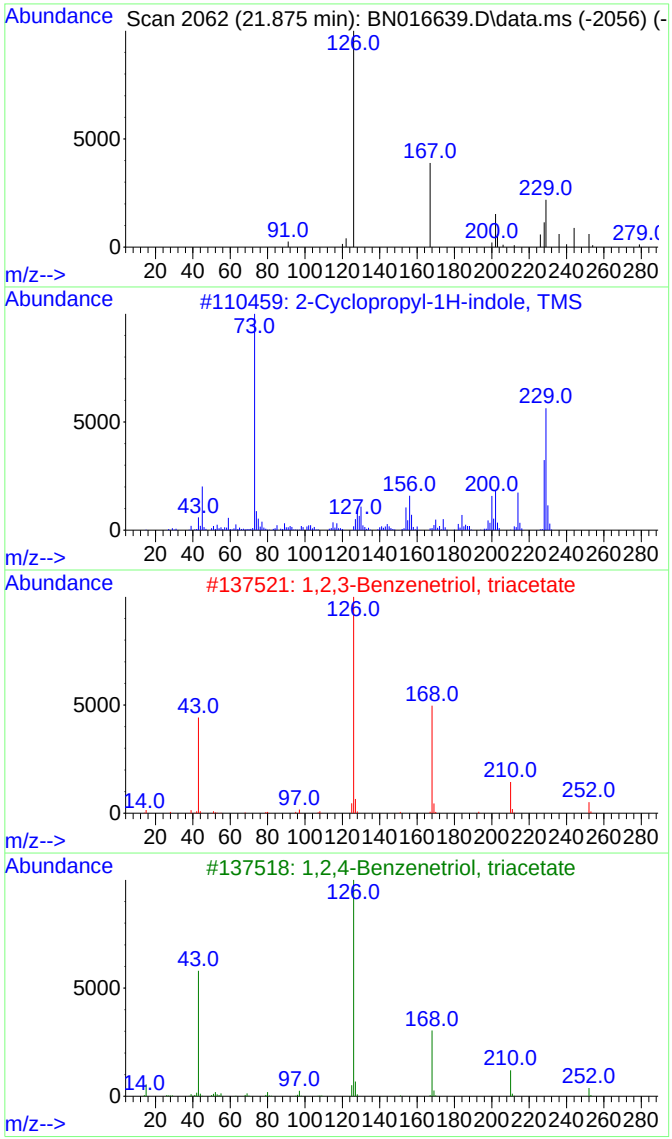
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

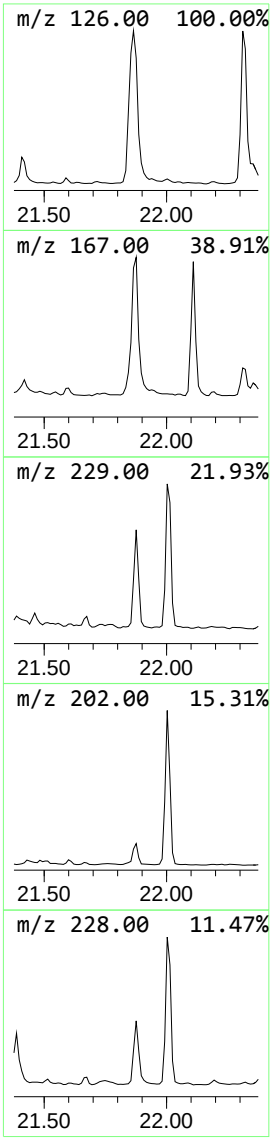
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 2-Cyclopropyl-1H-indole, TMS Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.875	0.30 ng	253314	Chrysene-d12	21.227

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclopropyl-1H-indole, TMS	229	C14H19NSi	1000494-09-0	5
2	1,2,3-Benzenetriol, triacetate	252	C12H12O6	000525-52-0	4
3	1,2,4-Benzenetriol, triacetate	252	C12H12O6	000613-03-6	4
4	Phloroglucinol triacetate	252	C12H12O6	002999-40-8	4
5	4-Morpholinopiperidine, N-(2-met...	240	C13H24N2O2	1010469-51-1	4





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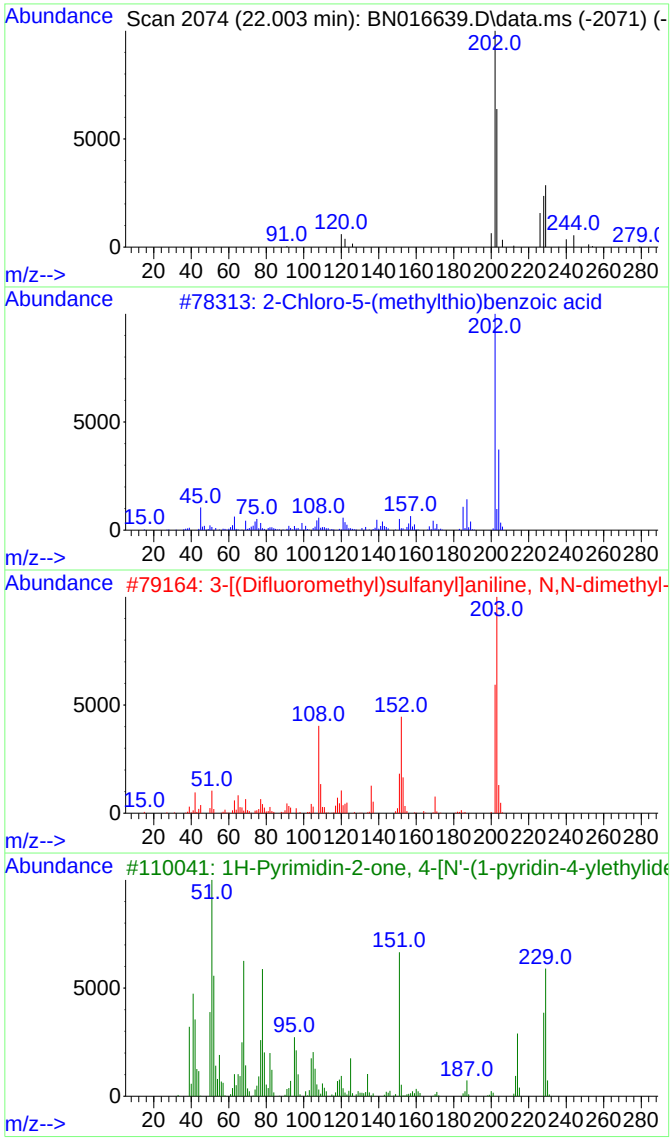
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

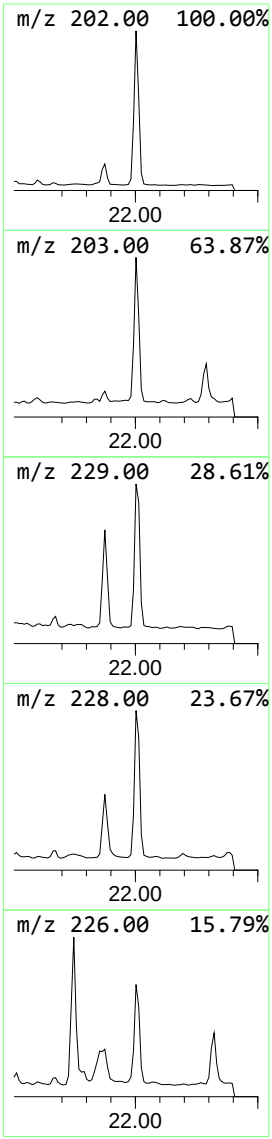
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 2-Chloro-5-(methylthio)benz... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.003	0.22 ng	192378	Chrysene-d12	21.227

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Chloro-5-(methylthio)benzoic acid	202	C8H7ClO2S	051546-12-4	7
2	3-[(Difluoromethyl)sulfanyl]anil...	203	C9H11F2NS	1000505-37-1	7
3	1H-Pyrimidin-2-one, 4-[N'-(1-pyr...	229	C11H11N5O	1000304-67-8	7
4	Pyridine, 2-chloro-6-(4-methylph...	203	C12H10ClN	1010380-55-1	5
5	2,4-Dichloro-3-methylaniline, N,...	203	C9H11Cl2N	1000511-94-6	5





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Data File : BN016639.D
Acq On : 01 Oct 2021 17:08
Operator : CG/JU
Sample : M4020-17
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-821-N-SO-2-2.5-093021

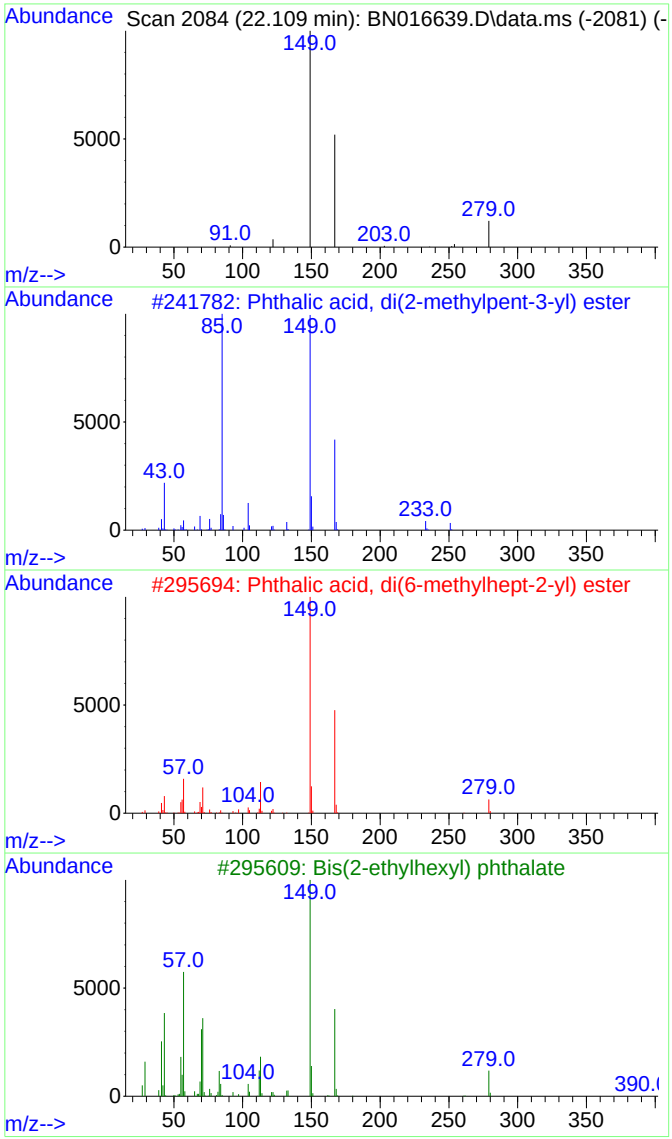
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

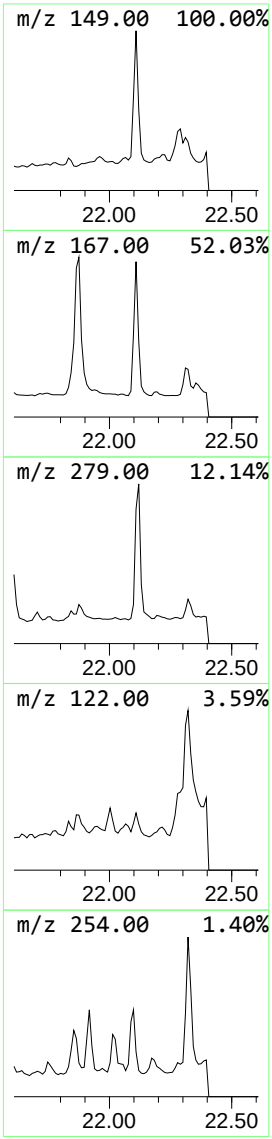
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 Phthalic acid, di(2-methylp... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.109	0.09 ng	75392	Chrysene-d12	21.227

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic acid, di(2-methylpent-3...	334	C20H30O4	1000356-92-3	9
2	Phthalic acid, di(6-methylhept-2...	390	C24H38O4	1000377-97-3	9
3	Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	9
4	4H-Thieno[3,2-b]pyrrole-5-carbox...	167	C7H5NO2S	039793-31-2	5
5	Nicotinic acid, 1,2-dihydro-4,6-...	167	C8H9NO3	024667-09-2	5





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Acq On : 01 Oct 2021 17:08
Operator : CG/JU
Sample : M4020-17
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : S-821-N-SO-2-2.5-093021

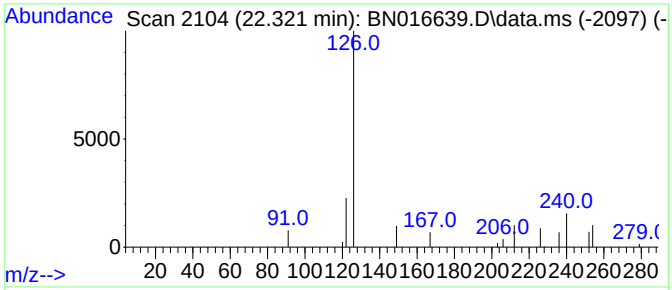
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

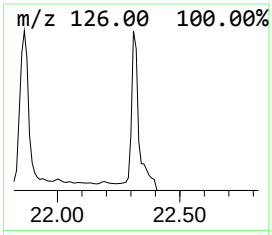
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

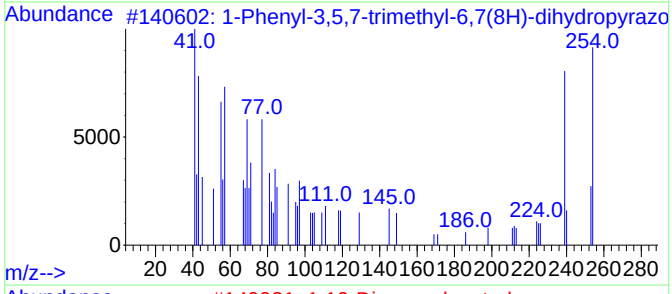
****
Peak Number 16 1-Phenyl-3,5,7-trimethyl-6,... Concentration Rank 6

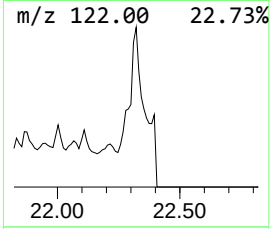
R.T.	EstConc	Area	Relative to ISTD	R.T.
22.321	0.32 ng	277325	Chrysene-d12	21.227

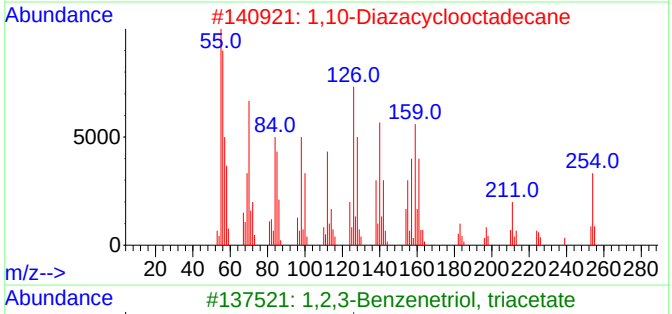
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenyl-3,5,7-trimethyl-6,7(8H)...	254	C15H18N4	064899-23-6	9
2	1,10-Diazacyclooctadecane	254	C16H34N2	000296-30-0	5
3	1,2,3-Benzenetriol, triacetate	252	C12H12O6	000525-52-0	4
4	1,2,4-Benzenetriol, triacetate	252	C12H12O6	000613-03-6	4
5	(3aR,3bS,6S,6aR,6bS)-6-Isopropyl...	206	C14H22O	013844-03-6	4

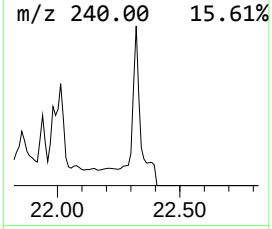


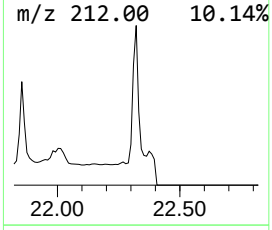


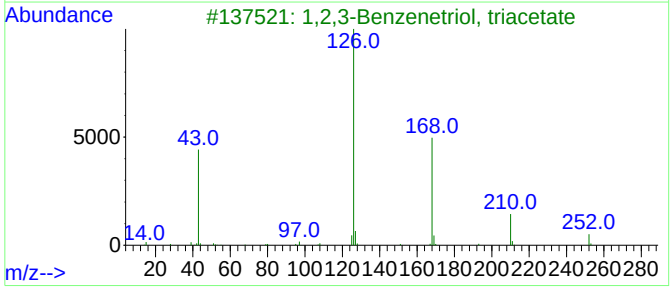


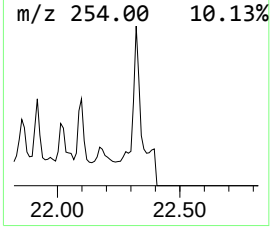












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Data File : BN016639.D
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Sample : M4020-17
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-821-N-SO-2-2.5-093021

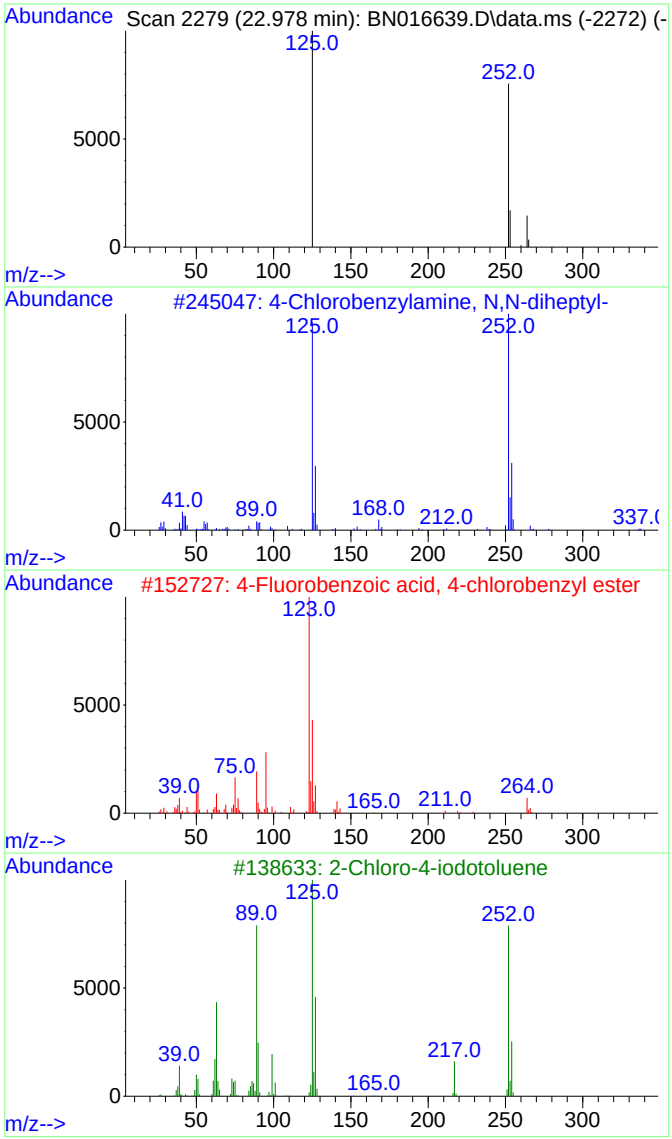
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

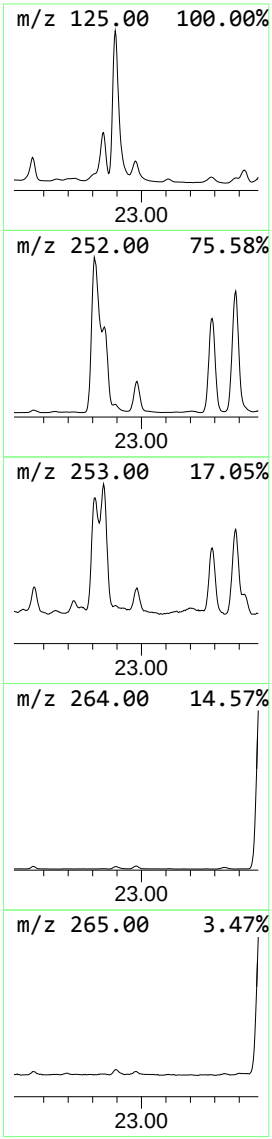
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 17 4-Chlorobenzylamine, N,N-di... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.978	0.08 ng	48035	Perylene-d12	23.485

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chlorobenzylamine, N,N-diheptyl-	337	C21H36ClN	1000310-39-1	9
2	4-Fluorobenzoic acid, 4-chlorobe...	264	C14H10ClFO2	1010279-92-4	7
3	2-Chloro-4-iodotoluene	252	C7H6ClI	083846-48-4	7
4	Sulphenone	252	C12H9ClO2S	000080-00-2	5
5	Naphthalene, 1-chloro-2,4-dinitro-	252	C10H5ClN2O4	002401-85-6	5





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ClientSampleId :
S-821-N-SO-2-2.5-093021

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

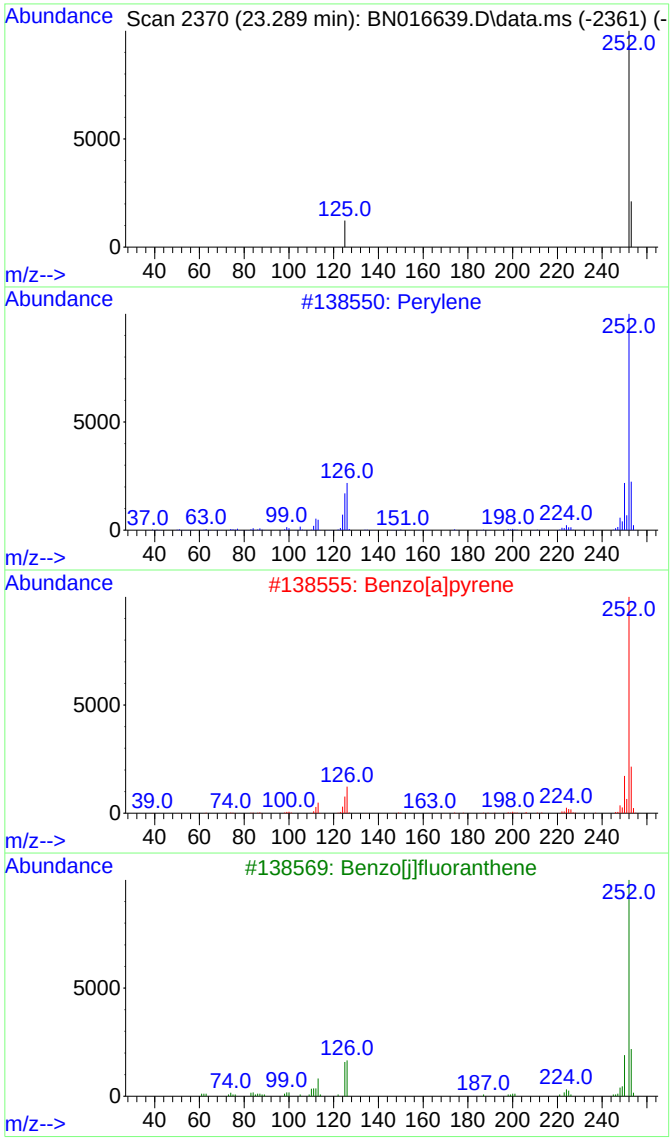
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

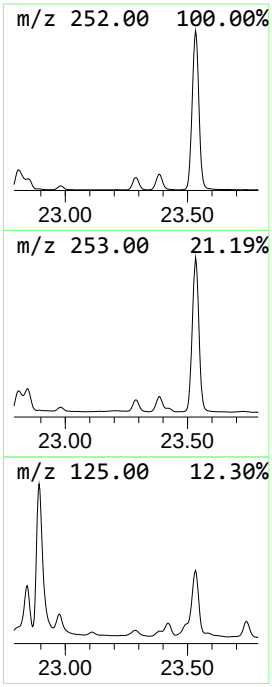
****

Peak Number 18 Perylene Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.290	0.09 ng	51829	Perylene-d12	23.485

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	9
2	Benzo[a]pyrene	252	C20H12	000050-32-8	9
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	9
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	9
5	Benzo[b]fluoranthene	252	C20H12	000205-99-2	9





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Acq On : 01 Oct 2021 17:08
Operator : CG/JU
Sample : M4020-17
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-821-N-SO-2-2.5-093021

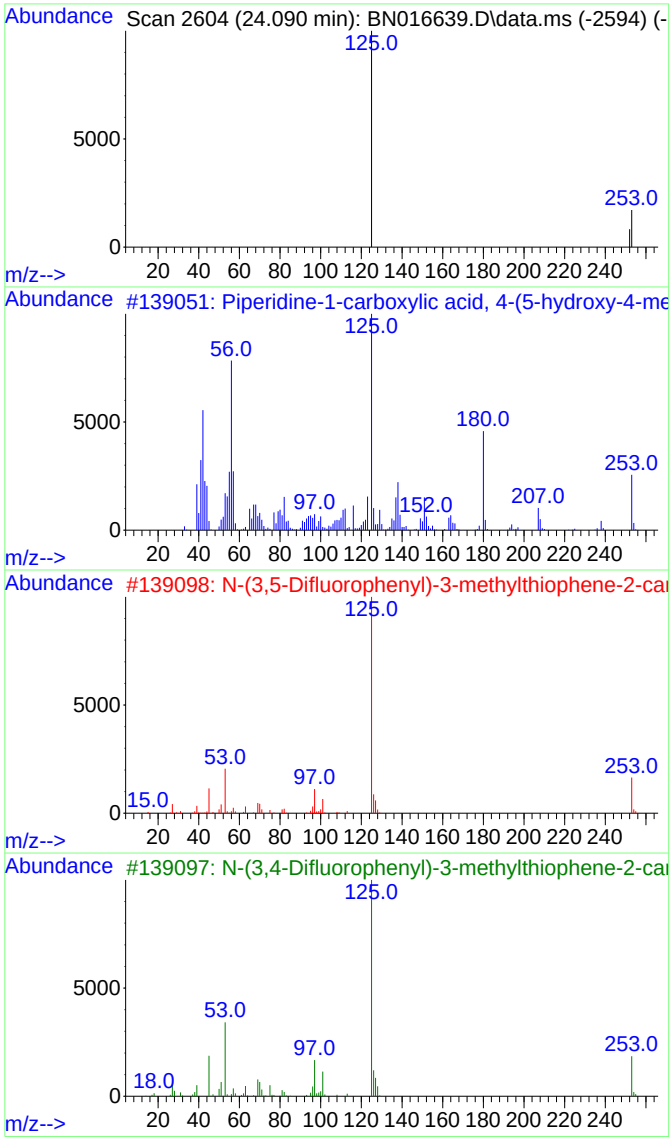
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

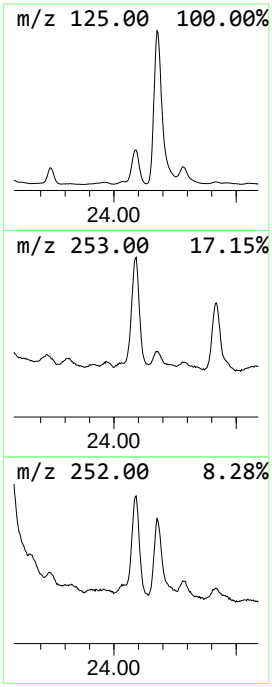
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 19 Piperidine-1-carboxylic aci... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.090	0.10 ng	57038	Perylene-d12	23.485

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Piperidine-1-carboxylic acid, 4-...	253	C12H19N3O3	1000316-66-8	5
2	N-(3,5-Difluorophenyl)-3-methylt...	253	C12H9F2NOS	1000436-25-2	4
3	N-(3,4-Difluorophenyl)-3-methylt...	253	C12H9F2NOS	1000436-25-1	4
4	Furane-2-carboxylic acid, 5-(3-c...	252	C12H9ClO4	074556-56-2	4
5	Cyclohexanecarboxylic acid, 4-ch...	252	C14H17ClO2	1000279-91-6	4





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Sample : M4020-17
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-821-N-SO-2-2.5-093021

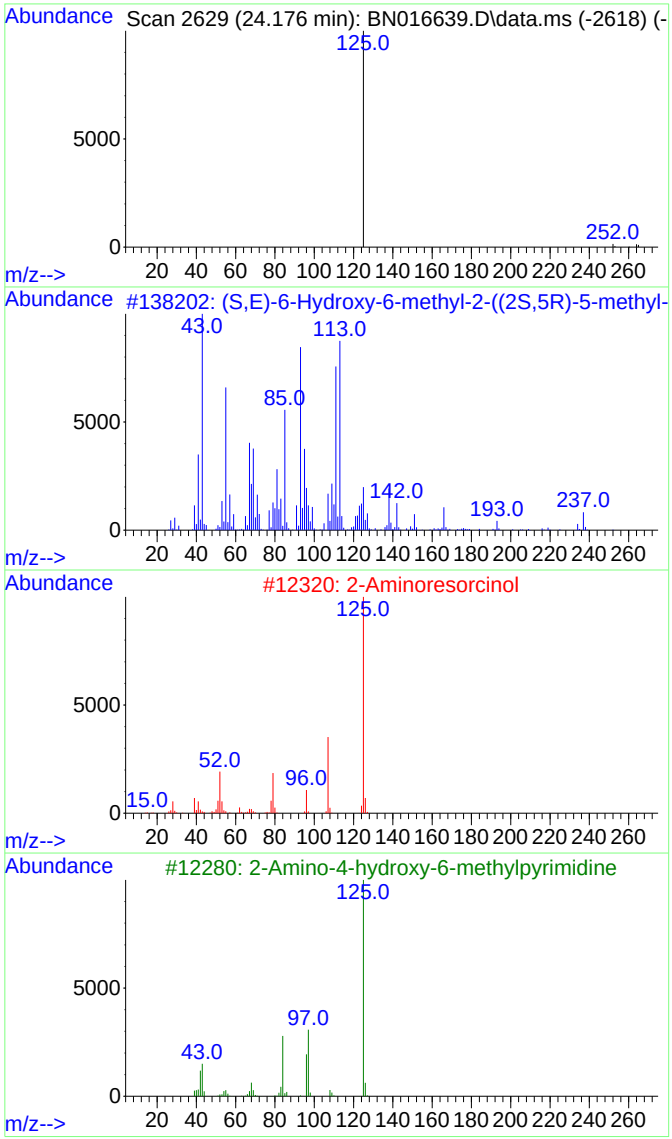
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

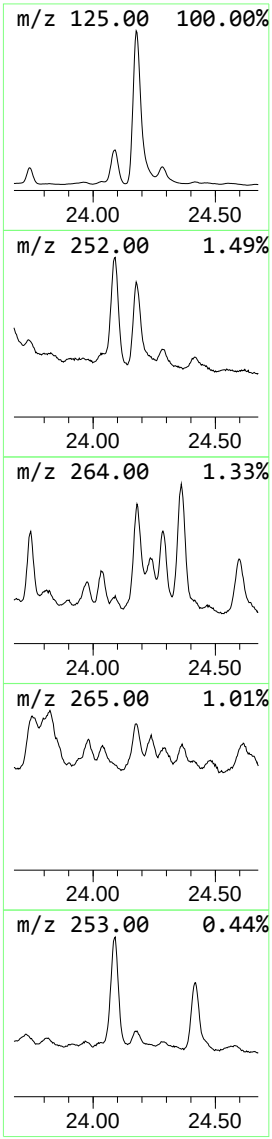
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 20 (S,E)-6-Hydroxy-6-methyl-2-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.176	0.42 ng	243366	Perylene-d12	23.485

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S,E)-6-Hydroxy-6-methyl-2-((2S,...	252	C15H24O3	088243-64-5	3
2	2-Aminoresorcinol	125	C6H7NO2	003163-15-3	2
3	2-Amino-4-hydroxy-6-methylpyrimi...	125	C5H7N3O	003977-29-5	2
4	2(1H)-Pyrimidinone, 4-amino-5-me...	125	C5H7N3O	000554-01-8	2
5	2,4-Diamino-6-methyl-1,3,5-triazine	125	C4H7N5	000542-02-9	2





Tentatively Identified Compound (LSC) summary

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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
beta-Alanine amide	3.502	0.1	ng	29959	1	7.643	102039	0.4
Butane	4.821	1.0	ng	261725	1	7.643	102039	0.4
Butane	7.938	1.5	ng	384061	1	7.643	102039	0.4
2-Oxazolidinone...	10.191	0.3	ng	130693	2	10.407	182024	0.4
Vanillin	13.178	0.5	ng	242496	3	14.269	207501	0.4
1-Pentanone, 1-...	14.523	0.1	ng	69566	3	14.269	207501	0.4
2,2-Diphenyleth...	16.007	0.4	ng	179481	4	17.018	192024	0.4
2-Mercapto-3-(t...	17.225	0.1	ng	48543	4	17.018	192024	0.4
2,6-Dichloro-3-...	17.784	0.2	ng	98276	4	17.018	192024	0.4
1-Cyclohexene-1...	17.918	0.1	ng	41519	4	17.018	192024	0.4
2(1H)-Pyridinet...	17.955	0.1	ng	62814	4	17.018	192024	0.4
Butanoic acid, ...	20.973	0.2	ng	195740	5	21.227	343179	0.4
2-Cyclopropyl-1...	21.875	0.3	ng	253314	5	21.227	343179	0.4
2-Chloro-5-(met...	22.003	0.2	ng	192378	5	21.227	343179	0.4
Phthalic acid, ...	22.109	0.1	ng	75392	5	21.227	343179	0.4
1-Phenyl-3,5,7-...	22.321	0.3	ng	277325	5	21.227	343179	0.4
4-Chlorobenzyla...	22.978	0.1	ng	48035	6	23.485	229613	0.4
Perylene	23.290	0.1	ng	51829	6	23.485	229613	0.4
Piperidine-1-ca...	24.090	0.1	ng	57038	6	23.485	229613	0.4
(S,E)-6-Hydroxy...	24.176	0.4	ng	243366	6	23.485	229613	0.4