LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101321\
Data File : BM032503.D
Acq On : 13 Oct 2021 19:29
Operator : CG/JU
Sample : M4142-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 2087

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_M\Methods\8270-BM100221.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM032503.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.249	63	70	75	rBV2	240888	322741	2.09%	0.197%
2	3.313	75	81	86	rBV2	257412	551946	3.57%	0.338%
3	3.637	131	136	140	rBV2	147107	261099	1.69%	0.160%
4	3.731	140	152	155	rBV2	294682	721924	4.67%	0.442%
5	4.013	196	200	207	rBV	153393	245794	1.59%	0.150%
6	4.107	212	216	226	rVB2	130718	261183	1.69%	0.160%
7	4.690	310	315	320	rVV	192025	266769	1.72%	0.163%
8	4.755	320	326	337	rVB4	108276	236092	1.53%	0.144%
9	5.096	375	384	392	rVV2	255543	558750	3.61%	0.342%
10	5.184	392	399	405	rVV	2565252	3774144	24.40%	2.308%
11	5.996	532	537	549	rVB	155497	272917	1.76%	0.167%
12	6.143	557	562	570	rVB3	545180	1124984	7.27%	0.688%
13	6.254	576	581	586	rBV	296278	409941	2.65%	0.251%
14	6.690	650	655	664	rVV2	345779	629848	4.07%	0.385%
15	6.801	667	674	684	rBV	1534843	2512475	16.25%	1.537%
16	7.337	760	765	770	rBV	232612	333824	2.16%	0.204%
17	7.396	770	775	779	rBV3	153330	278996	1.80%	0.171%
18	7.601	804	810	815	rBV2	782489	1251886	8.09%	0.766%
19	7.684	819	824	834	rBV	853047	1377213	8.91%	0.842%
20	7.848	843	852	855	rBV4	117569	268674	1.74%	0.164%
21	8.072	885	890	895	rBV	179288	277163	1.79%	0.170%
22	8.125	895	899	908	rVB	142788	270525	1.75%	0.165%
23	8.395	939	945	956	rVB3	293095	884839	5.72%	0.541%
24	8.707	972	998	1001	rBV	2805513	12313631	79.62%	7.531%
25	8.742	1002	1004	1005	rVV	616274	447301	2.89%	0.274%
26	9.060	1042	1058	1061	rBV	872582	3046864	19.70%	1.864%
27	9.142	1067	1072	1083	rVB3	400242	916828	5.93%	0.561%
28	9.319	1094	1102	1108	rBV4	185416	347624	2.25%	0.213%
29	9.595	1145	1149	1157	rBV3	173367	350452	2.27%	0.214%
30	9.789	1165	1182	1188	rBV	580472	2149589	13.90%	1.315%
31	10.007	1211	1219	1225	rBV7	204237	536601	3.47%	0.328%
32	10.178	1239	1248	1257	rBV	622504	1196573	7.74%	0.732%
33	10.289	1258	1267	1273	rVV4	341167	840157	5.43%	0.514%
34	10.389	1273	1284	1289	rVV	982779	1686838	10.91%	1.032%
35	10.660	1325	1330	1336	rBV3	169731	312124	2.02%	0.191%
36	10.748	1337	1345	1351	rVB7	91662	294472	1.90%	0.180%

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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
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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 >
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Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	10.936	1367	1377	1381	rBV	1341292	2410555	15.59%	1.474%
38	10.995	1381	1387	1390	rVV2	1138055	2444008	15.80%	1.495%
39	11.031	1390	1393	1401	rVB	1193976	1886978	12.20%	1.154%
40	11.236	1424	1428	1431	rBV3	175594	307160	1.99%	0.188%
41	11.413	1454	1458	1461	rBV2	223692	446303	2.89%	0.273%
42	11.460	1462	1466	1482	rVB9	863404	3433909	22.20%	2.100%
43	11.619	1490	1493	1498	rVB4	236750	322494	2.09%	0.197%
44	11.701	1503	1507	1510	rVV3	235758	397004	2.57%	0.243%
45	11.766	1513	1518	1530	rVB3	491876	1223485	7.91%	0.748%
46	11.866	1530	1535	1542	rBV5	187005	476707	3.08%	0.292%
47	12.272	1599	1604	1608	rBV2	334734	508402	3.29%	0.311%
48	12.325	1609	1613	1617	rVV4	307499	532515	3.44%	0.326%
49	12.389	1620	1624	1633	rVV4	413365	1177111	7.61%	0.720%
50	12.466	1634	1637	1644	rVB3	163931	347122	2.24%	0.212%
51	12.748	1670	1685	1690	rBV	4307276	13890461	89.82%	8.496%
52	12.795	1690	1693	1696	rVV	1019820	1387526	8.97%	0.849%
53	12.866	1700	1705	1711	rVV	5710793	8809846	56.97%	5.388%
54	12.919	1711	1714	1722	rVB	473193	664809	4.30%	0.407%
55	13.048	1730	1736	1742	rBV4	671588	1389758	8.99%	0.850%
56	13.113	1743	1747	1750	rBV2	236332	398142	2.57%	0.244%
57	13.183	1750	1759	1771	rVB	7572497	15465307	100.00%	9.459%
58	13.289	1771	1777	1781	rBV4	675034	1219048	7.88%	0.746%
59	13.372	1788	1791	1794	rBV	283208	335740	2.17%	0.205%
60	13.419	1794	1799	1803	rVB4	621552	953360	6.16%	0.583%
61	13.519	1812	1816	1818	rBV	252211	374653	2.42%	0.229%
62	13.548	1818	1821	1823	rVV3	206072	284650	1.84%	0.174%
63	13.689	1841	1845	1849	rVB3	273331	370603	2.40%	0.227%
64	13.760	1850	1857	1861	rVB8	151271	357201	2.31%	0.218%
65	13.819	1862	1867	1874	rVB5	456317	919124	5.94%	0.562%
66	13.919	1874	1884	1891	rBV6	1045429	2913658	18.84%	1.782%
67	13.977	1891	1894	1897	rVV	458383	559177	3.62%	0.342%
68	14.066	1905	1909	1918	rVB4	668202	1045821	6.76%	0.640%
69	14.248	1934	1940	1947	rBV	1763572	3133993	20.26%	1.917%
70	14.377	1959	1962	1964	rBV3	222101	292236	1.89%	0.179%
71	14.413	1964	1968	1972	rVV3	544434	984002	6.36%	0.602%
72	14.472	1972	1978	1987	rVB3	772803	1863358	12.05%	1.140%
73	14.566	1992	1994	2003	rVB4	295166	506396	3.27%	0.310%
74	14.666	2007	2011	2014	rBV3	280384	483847	3.13%	0.296%
75	14.772	2024	2029	2032	rBV5	201477	350657	2.27%	0.214%
76	14.836	2035	2040	2045	rVV	1935792	2986444	19.31%	1.827%

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Misc :
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Instrument : BNA_M
ClientSampleId : 2087

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
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Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	14.901	2048	2051	2056	rVB	437266	601182	3.89%	0.368%
78	15.077	2078	2081	2087	rVB4	366093	607708	3.93%	0.372%
79	15.136	2088	2091	2093	rBV	232499	271839	1.76%	0.166%
80	15.213	2101	2104	2110	rVB2	470509	701401	4.54%	0.429%
81	15.560	2160	2163	2167	rBV4	221722	354508	2.29%	0.217%
82	15.660	2177	2180	2184	rVB3	524135	645104	4.17%	0.395%
83	15.707	2186	2188	2189	rVV	289839	272616	1.76%	0.167%
84	15.742	2189	2194	2199	rVB	4024541	5688775	36.78%	3.479%
85	15.860	2206	2214	2218	rBV	3155365	5598188	36.20%	3.424%
86	15.995	2233	2237	2245	rVB4	337817	626989	4.05%	0.383%
87	16.066	2246	2249	2252	rBV3	212704	314600	2.03%	0.192%
88	16.977	2400	2404	2409	rBV	1595314	2186748	14.14%	1.337%
89	17.083	2418	2422	2428	rVB2	370517	632945	4.09%	0.387%
90	17.648	2514	2518	2524	rVB6	602145	867241	5.61%	0.530%
91	17.877	2550	2557	2563	rBV6	613988	1304835	8.44%	0.798%
92	18.095	2592	2594	2600	rVB	267307	311329	2.01%	0.190%
93	18.642	2685	2687	2693	rVB	468003	552500	3.57%	0.338%
94	19.077	2756	2761	2766	rVB	6159064	7356312	47.57%	4.499%
95	19.154	2771	2774	2782	rVB4	402656	703712	4.55%	0.430%
96	19.595	2844	2849	2854	rVB	7253863	9341754	60.40%	5.714%
97	20.071	2927	2930	2936	rVB	379444	411060	2.66%	0.251%
98	21.148	3108	3113	3118	rVB	1725150	2148129	13.89%	1.314%
99	21.265	3130	3133	3139	rVB	228773	281682	1.82%	0.172%
100	23.289	3471	3477	3485	rVB2	1368263	2334518	15.10%	1.428%

Sum of corrected areas: 163502026

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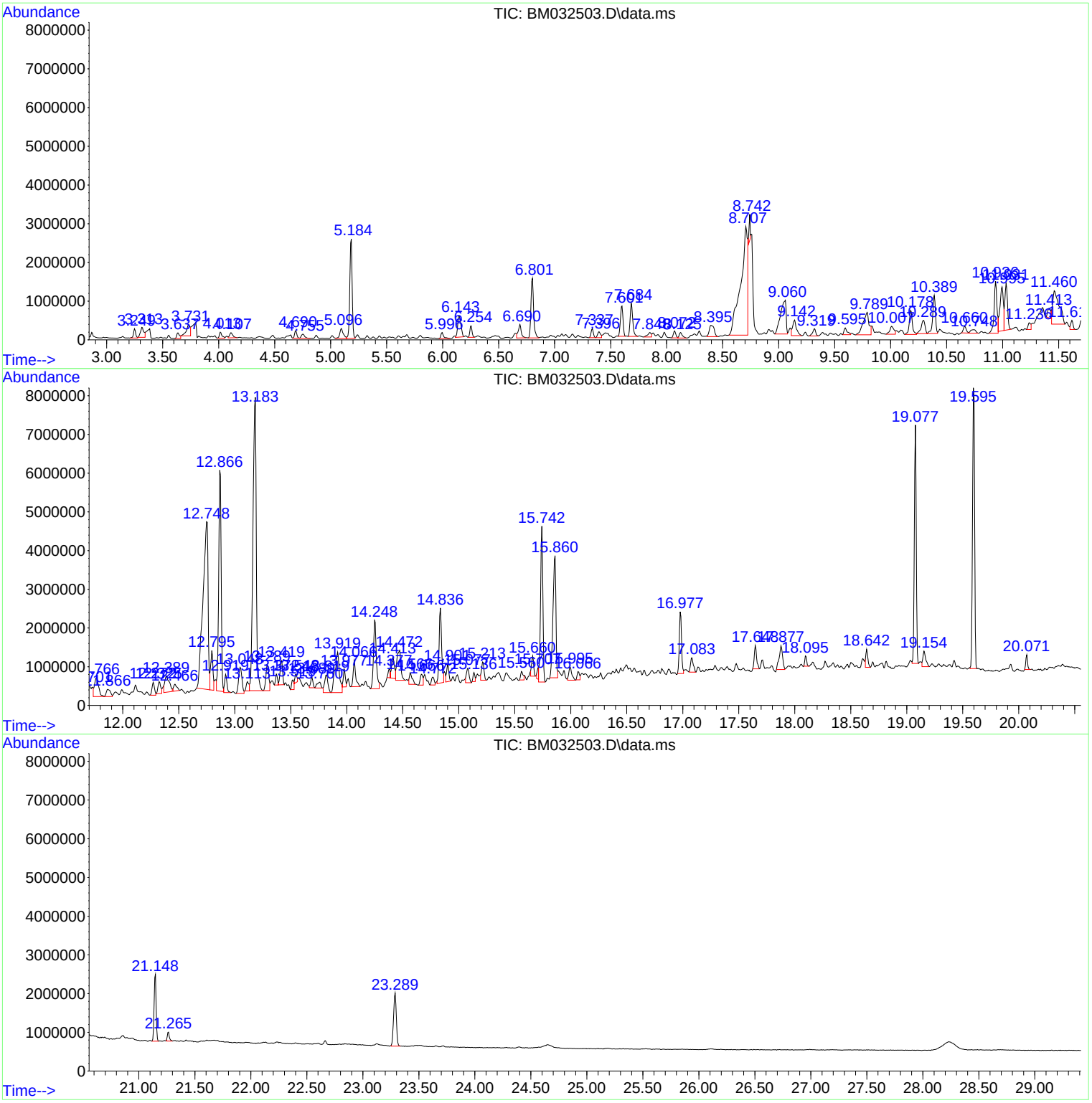
Instrument :
BNA_M
ClientSampleId :
2087

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.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_M\Data\BM101321\
Data File : BM032503.D
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Instrument : BNA_M
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

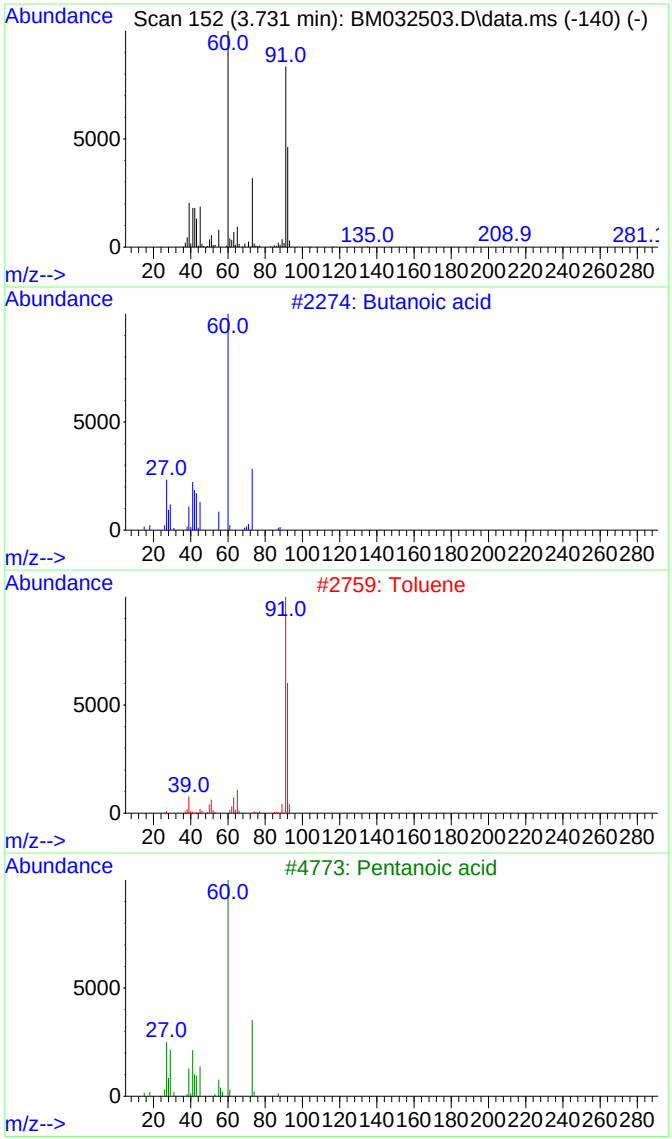
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

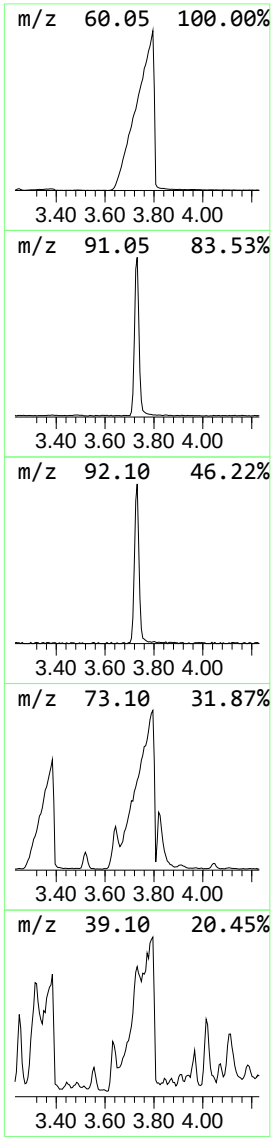
****

Peak Number 1 unknown3.731 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.731	11.53 ng	721924	1,4-Dichlorobenzene-d4	7.601

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid	88	C4H8O2	000107-92-6	49
2	Toluene	92	C7H8	000108-88-3	42
3	Pentanoic acid	102	C5H10O2	000109-52-4	38
4	1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	38
5	Butanoic acid, 4-chloro-	122	C4H7ClO2	000627-00-9	32





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101321\
Data File : BM032503.D
Acq On : 13 Oct 2021 19:29
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Sample : M4142-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 2087

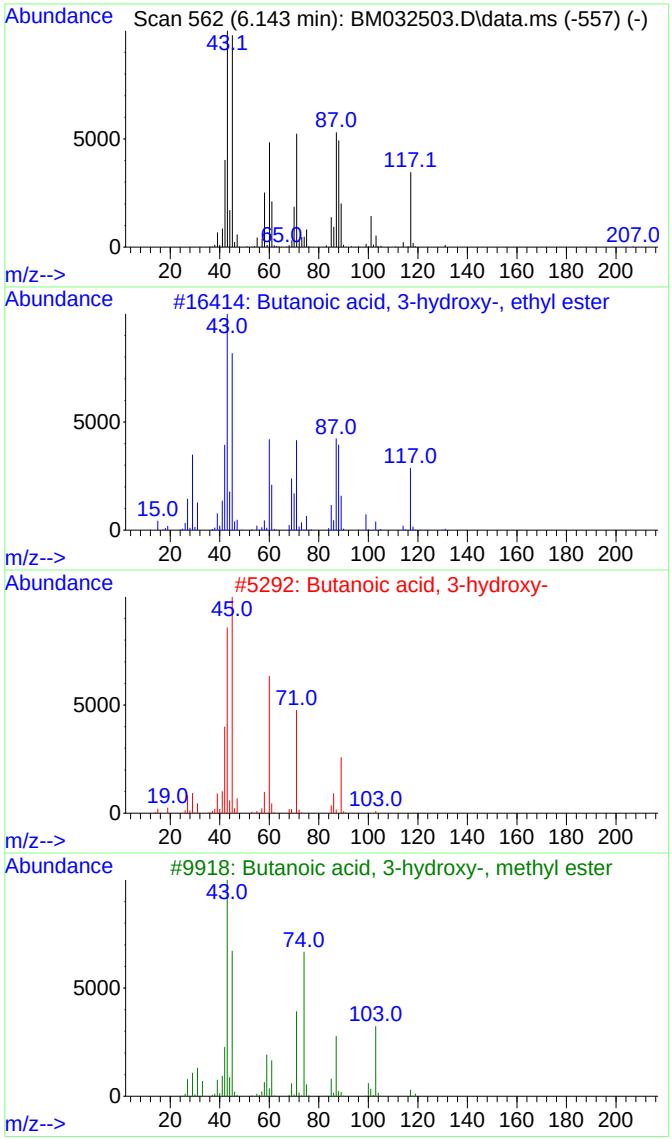
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

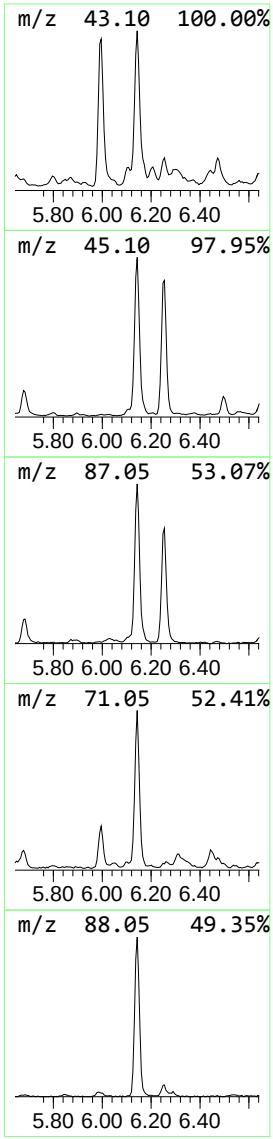
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butanoic acid, 3-hydroxy-, ... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.143	17.97 ng	1124980	1,4-Dichlorobenzene-d4	7.601

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 3-hydroxy-, ethyl...	132	C6H12O3	005405-41-4	91
2	Butanoic acid, 3-hydroxy-	104	C4H8O3	000300-85-6	43
3	Butanoic acid, 3-hydroxy-, methy...	118	C5H10O3	001487-49-6	40
4	Butanoic acid, 3-hydroxy-, methy...	118	C5H10O3	053562-86-0	38
5	Acetic acid	60	C2H4O2	000064-19-7	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101321\
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Instrument : BNA_M
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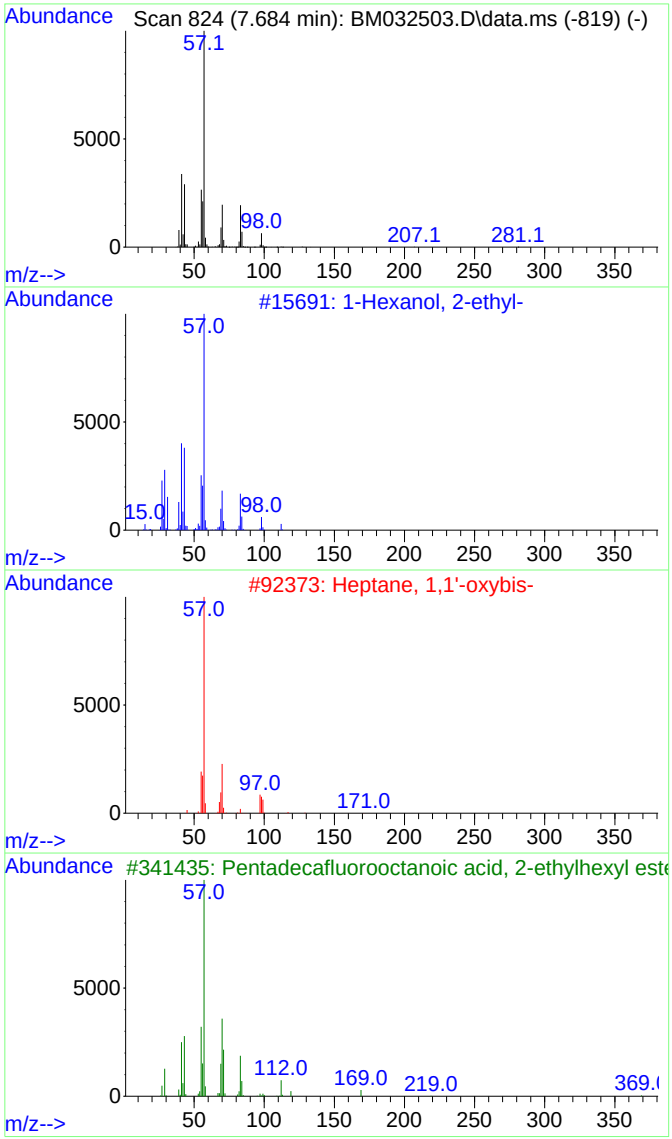
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

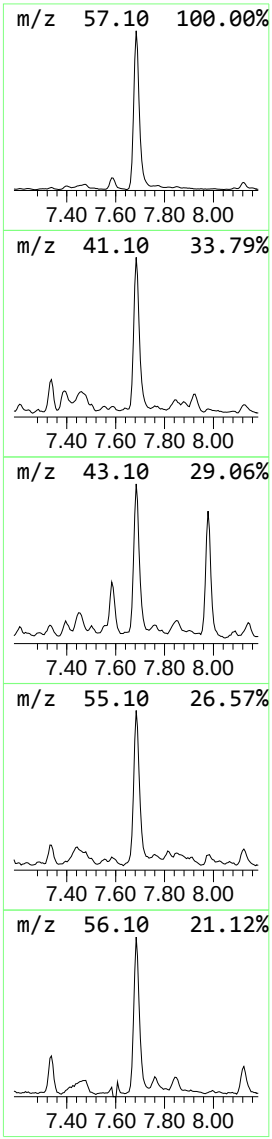
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.684	22.00 ng	1377210	1,4-Dichlorobenzene-d4	7.601

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	59
3	Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	47
4	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
5	Heptyl tetradecyl ether	312	C21H44O	1000406-39-3	39





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ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 2087

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

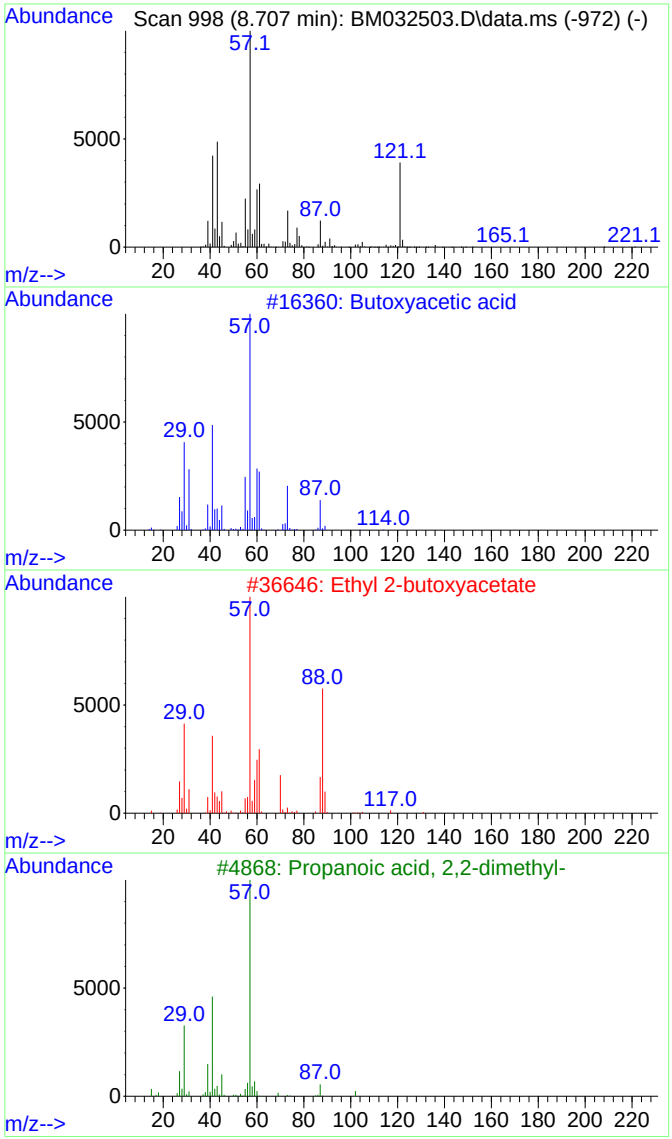
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

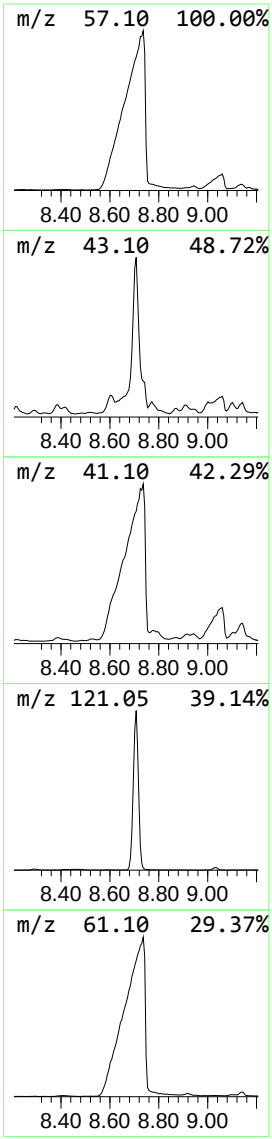
****

Peak Number 4 Butoxyacetic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.707	196.72 ng	12313600	1,4-Dichlorobenzene-d4	7.601

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butoxyacetic acid	132	C6H12O3	002516-93-0	72
2	Ethyl 2-butoxyacetate	160	C8H16O3	1000366-89-3	50
3	Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	27
4	Butanoic acid, 3,3-dimethyl-	116	C6H12O2	001070-83-3	27
5	Pentanoic acid, 4-methyl-	116	C6H12O2	000646-07-1	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101321\
Data File : BM032503.D
Acq On : 13 Oct 2021 19:29
Operator : CG/JU
Sample : M4142-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 2087

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

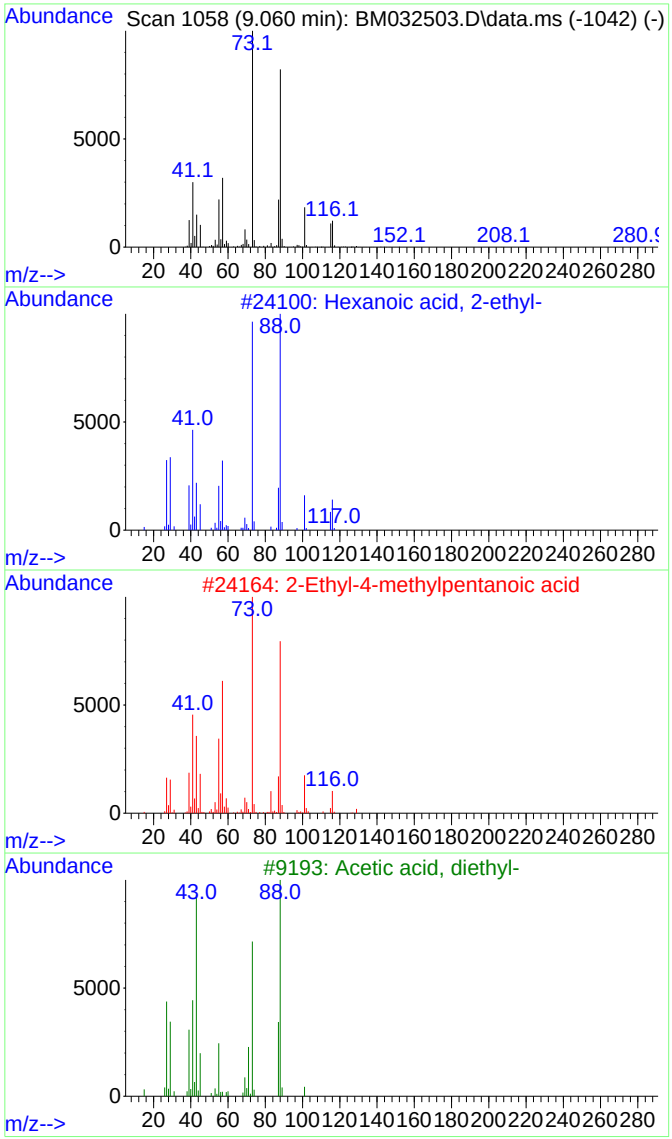
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

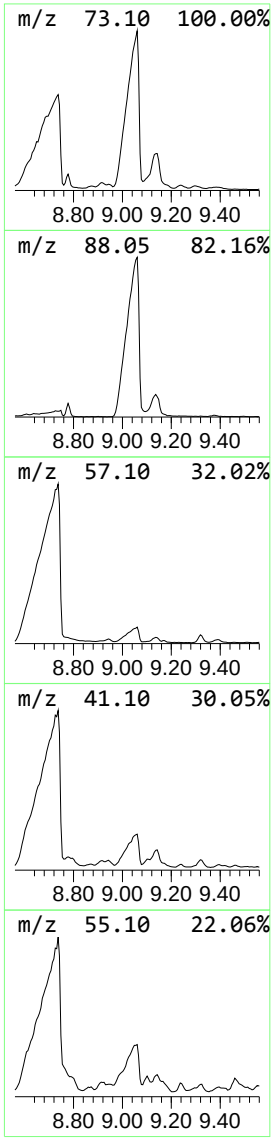
****

Peak Number 5 Hexanoic acid, 2-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.060	36.13 ng	3046860	Naphthalene-d8	10.389

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2	2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	72
3	Acetic acid, diethyl-	116	C6H12O2	000088-09-5	59
4	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	53
5	1,4-Dioxane	88	C4H8O2	000123-91-1	37





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Data File : BM032503.D
Acq On : 13 Oct 2021 19:29
Operator : CG/JU
Sample : M4142-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 2087

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

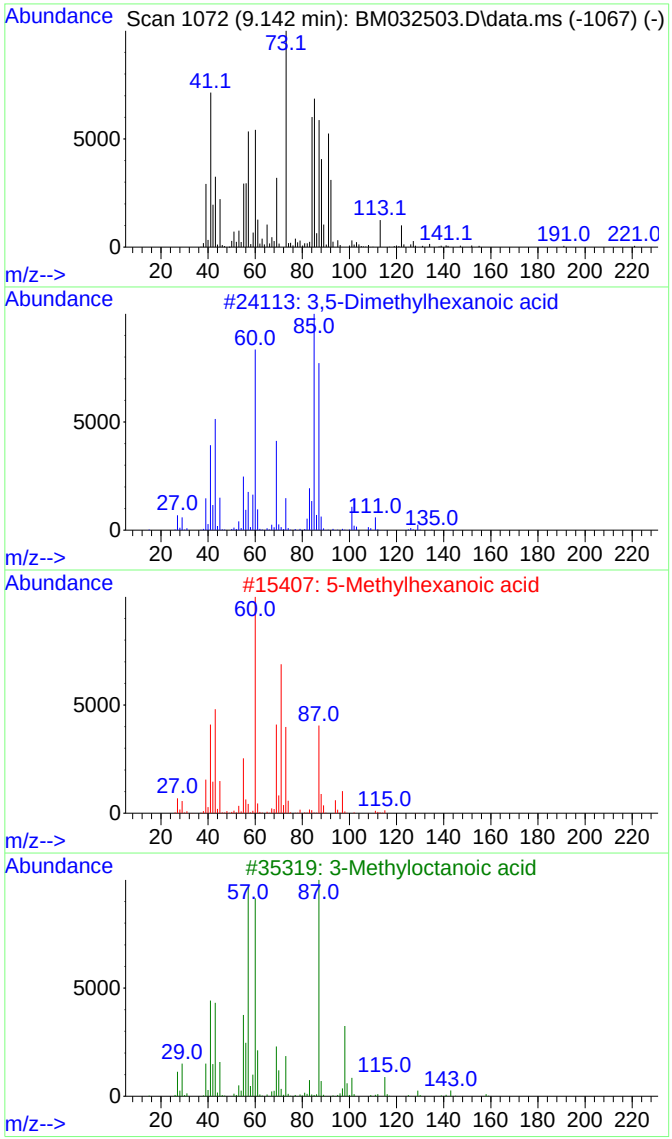
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

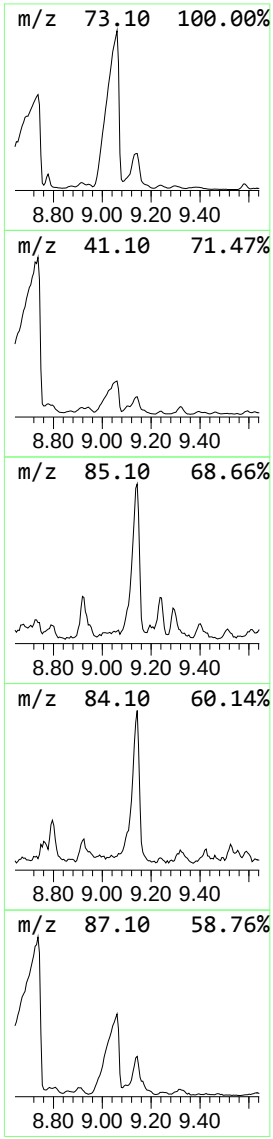
****

Peak Number 6 unknown9.142 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.142	10.87 ng	916828	Naphthalene-d8	10.389

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-Dimethylhexanoic acid	144	C8H16O2	060308-87-4	38
2	5-Methylhexanoic acid	130	C7H14O2	000628-46-6	35
3	3-Methyloctanoic acid	158	C9H18O2	006061-10-5	22
4	N-(5-Oxo-tetrahydro-furan-2-ylme...	157	C7H11NO3	1000188-71-2	22
5	3,4-Dimethylpentanoic acid	130	C7H14O2	003302-06-5	16





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Sample : M4142-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 2087

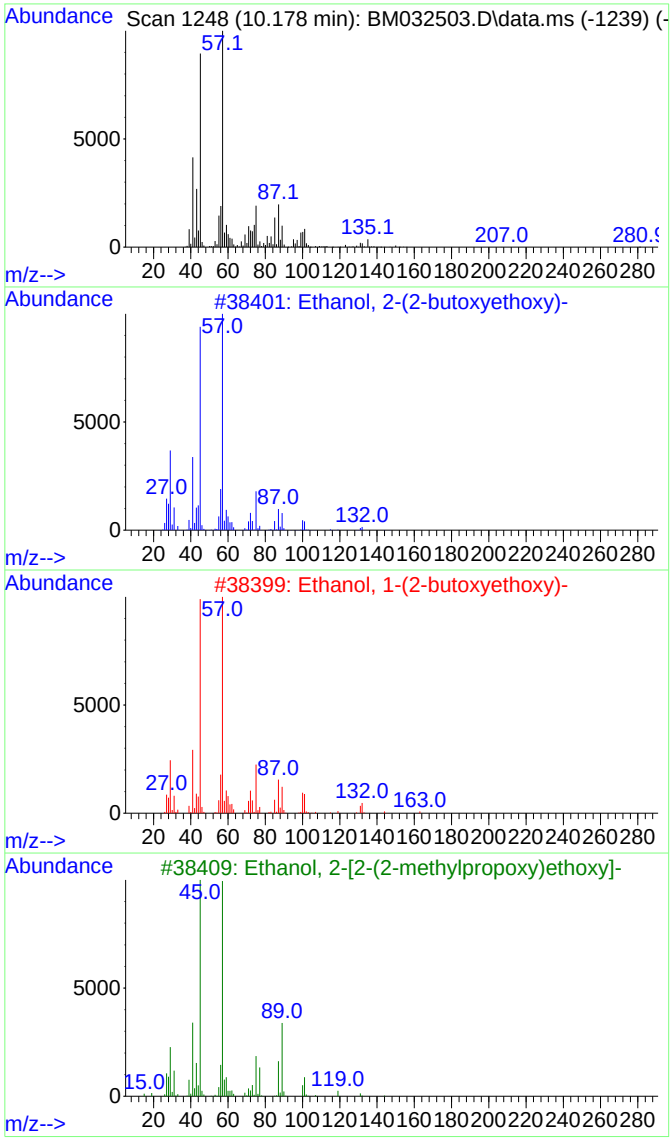
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

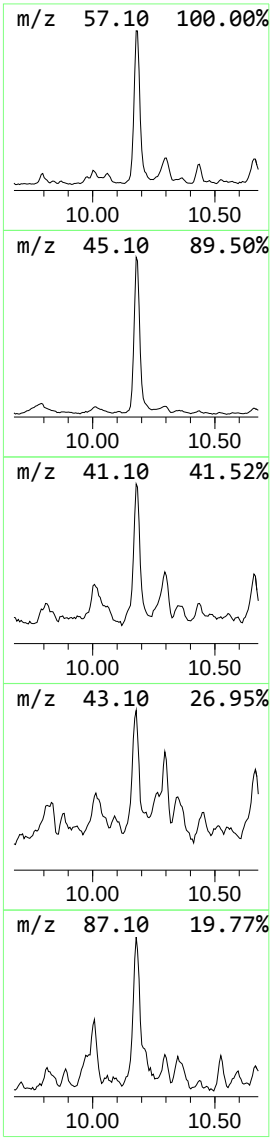
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.178	14.19 ng	1196570	Naphthalene-d8	10.389

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	86
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	78
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	72
4	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50
5	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50





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Operator : CG/JU
Sample : M4142-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 2087

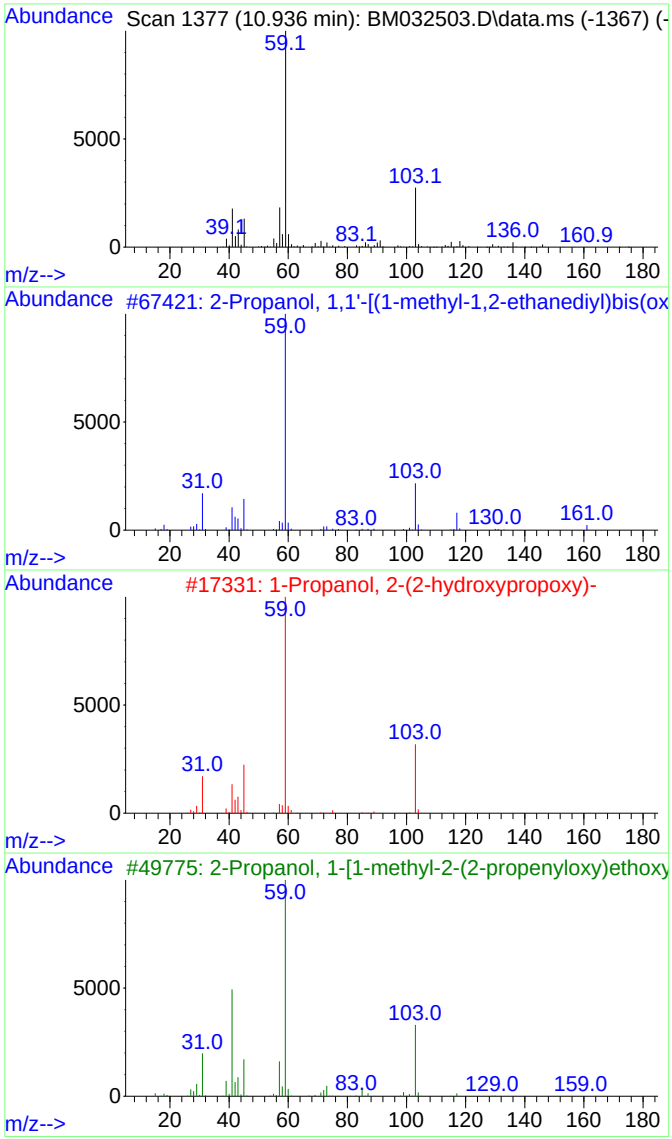
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

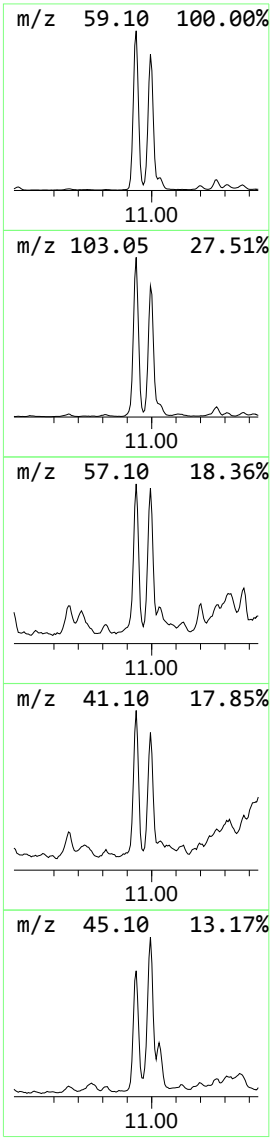
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 2-Propanol, 1,1'-[(1-methyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.937	28.58 ng	2410560	Naphthalene-d8	10.389

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1,1'-[(1-methyl-1,2-...	192	C9H20O4	001638-16-0	72
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72
3	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	64
4	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	64
5	Methane, diethoxy-	104	C5H12O2	000462-95-3	64





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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 2087

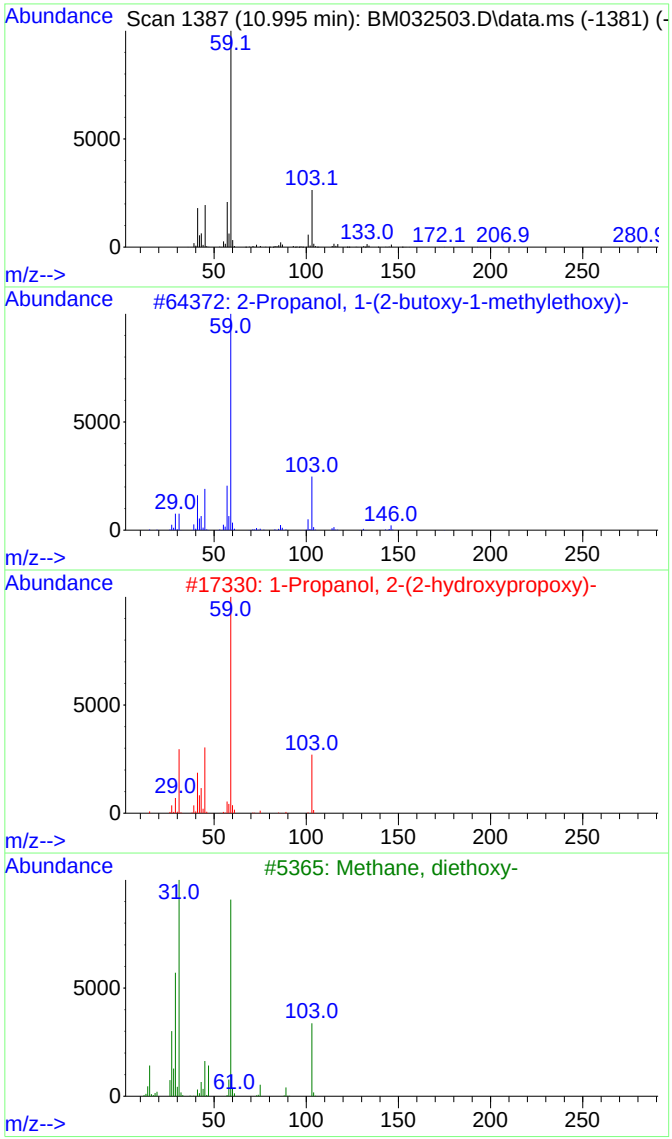
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

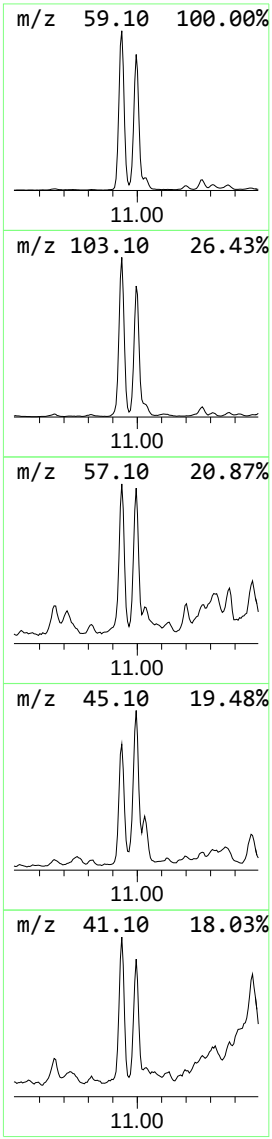
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 2-Propanol, 1-(2-butoxy-1-m... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.995	28.98 ng	2444010	Naphthalene-d8	10.389

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	86
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72
3	Methane, diethoxy-	104	C5H12O2	000462-95-3	64
4	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	64
5	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	56





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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 2087

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

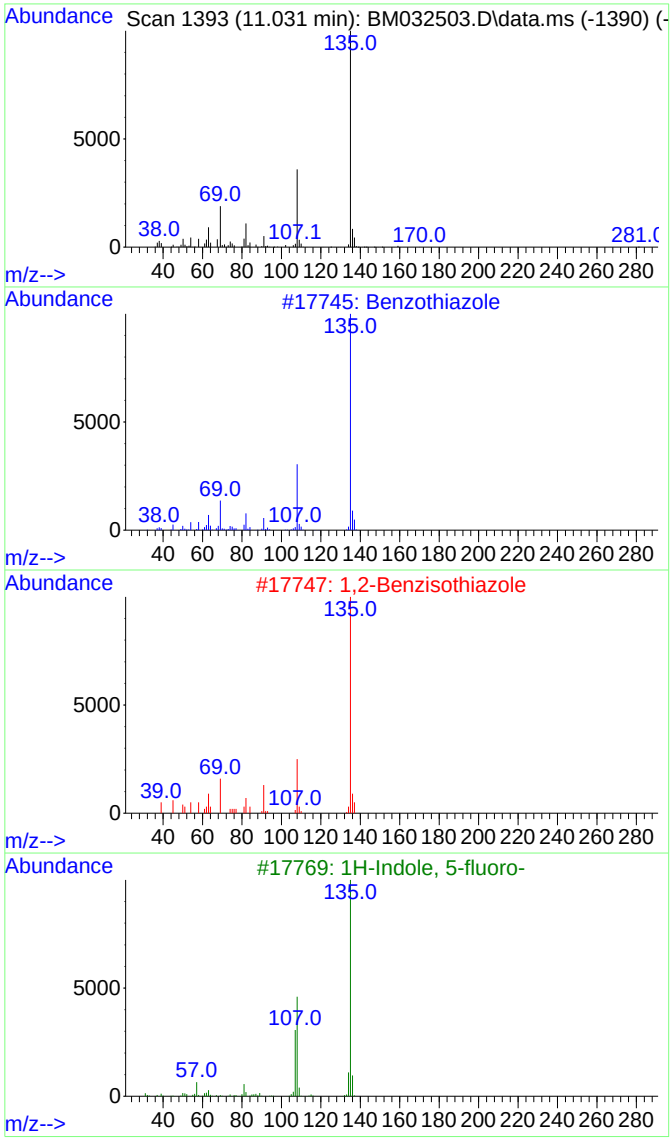
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

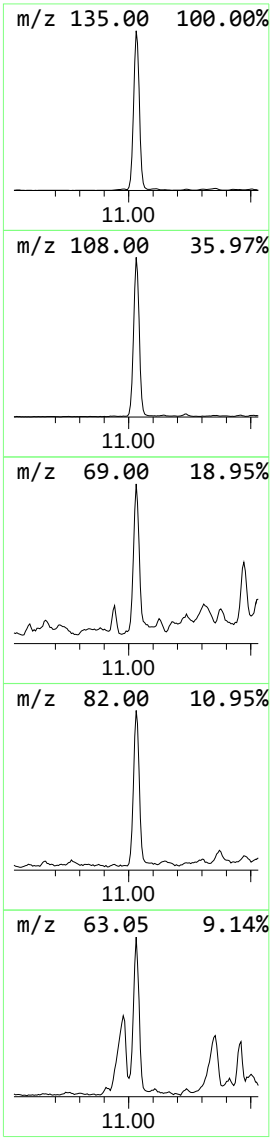
****

Peak Number 10 Benzothiazole Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.031	22.37 ng	1886980	Naphthalene-d8	10.389

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzothiazole	135	C7H5NS	000095-16-9	95
2	1,2-Benzisothiazole	135	C7H5NS	000272-16-2	90
3	1H-Indole, 5-fluoro-	135	C8H6FN	000399-52-0	64
4	1H-Pyrazolo[3,4-d]pyrimidin-4-amine	135	C5H5N5	002380-63-4	58
5	Adenine	135	C5H5N5	000073-24-5	53





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Acq On : 13 Oct 2021 19:29
Operator : CG/JU
Sample : M4142-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 2087

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

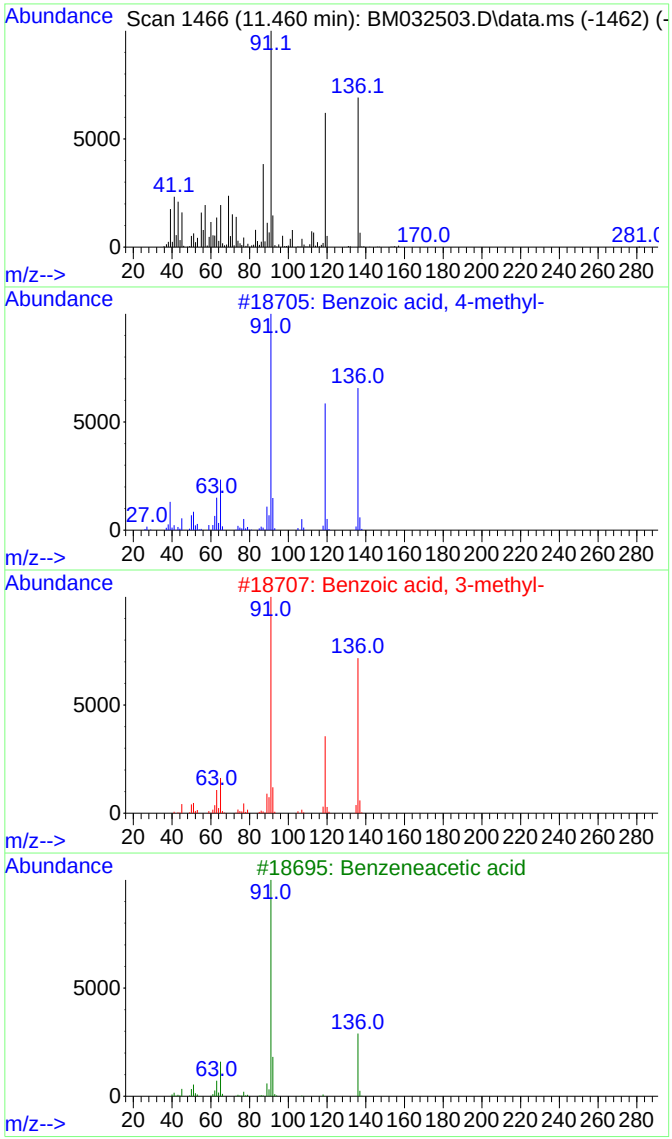
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

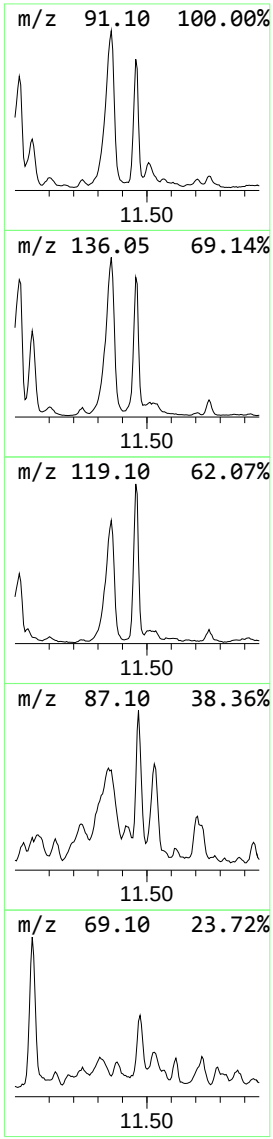
****

Peak Number 11 Benzoic acid, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.460	40.71 ng	3433910	Naphthalene-d8	10.389

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	96
2	Benzoic acid, 3-methyl-	136	C8H8O2	000099-04-7	60
3	Benzeneacetic acid	136	C8H8O2	000103-82-2	46
4	Benzoyl chloride, 4-methyl-	154	C8H7ClO	000874-60-2	38
5	m-Toluamide	135	C8H9NO	000618-47-3	35





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Acq On : 13 Oct 2021 19:29
Operator : CG/JU
Sample : M4142-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 2087

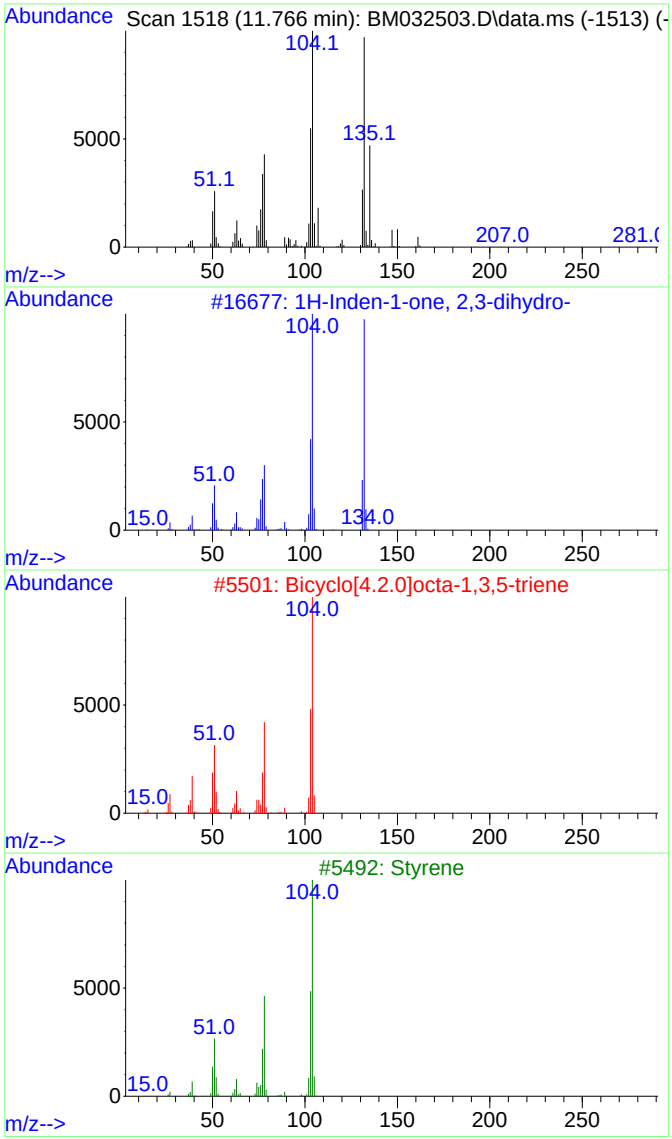
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

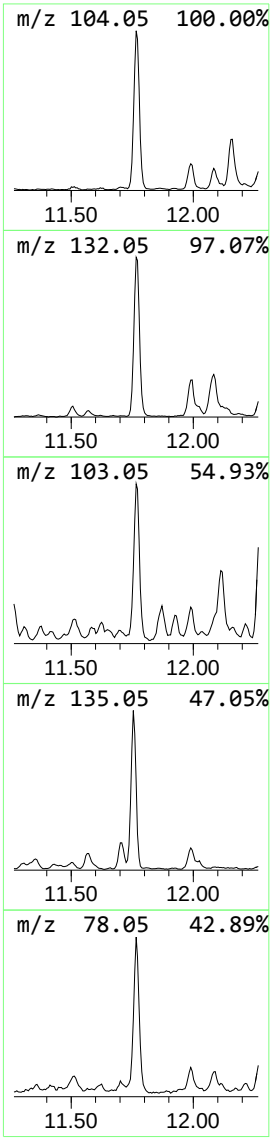
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 1H-Inden-1-one, 2,3-dihydro- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.766	14.51 ng	1223490	Naphthalene-d8	10.389

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Inden-1-one, 2,3-dihydro-	132	C9H8O	000083-33-0	93
2	Bicyclo[4.2.0]octa-1,3,5-triene	104	C8H8	000694-87-1	55
3	Styrene	104	C8H8	000100-42-5	55
4	2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	53
5	Benzofuran, 7-methyl-	132	C9H8O	017059-52-8	49





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Sample : M4142-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 2087

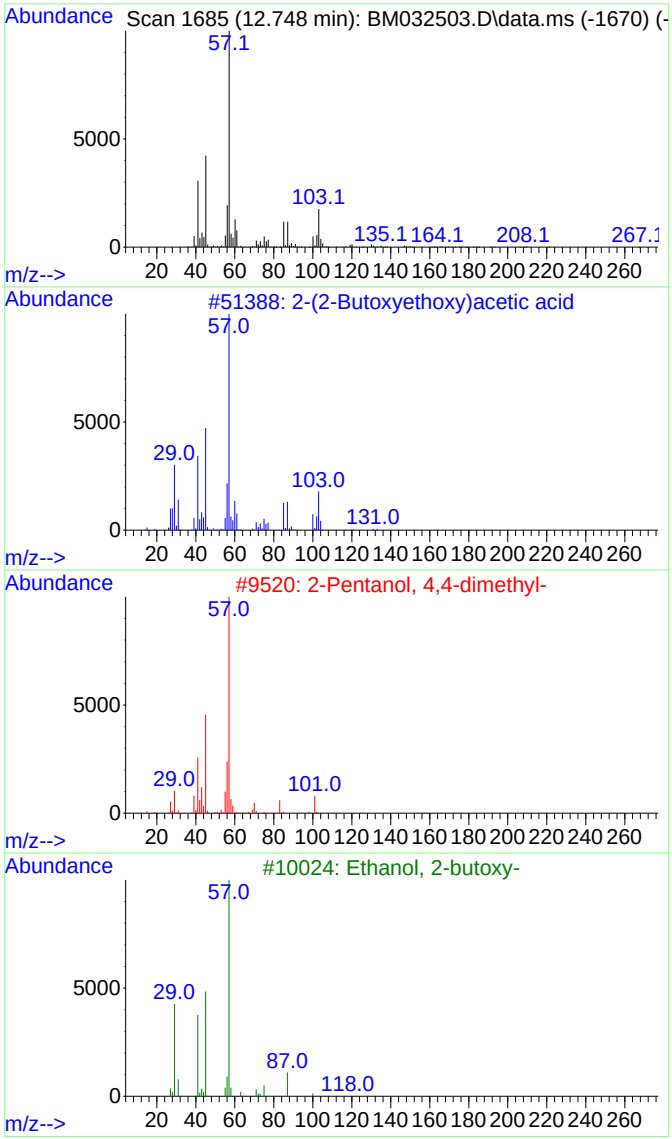
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

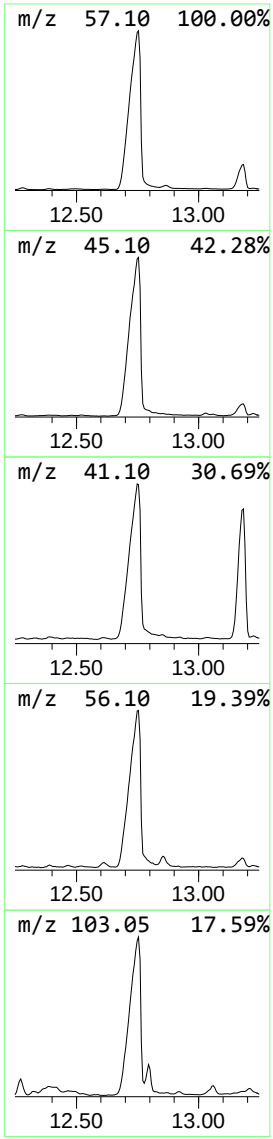
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 2-(2-Butoxyethoxy)acetic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.748	88.64 ng	13890500	Acenaphthene-d10	14.254

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(2-Butoxyethoxy)acetic acid	176	C8H16O4	082941-26-2	90
2	2-Pentanol, 4,4-dimethyl-	116	C7H16O	006144-93-0	47
3	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	43
4	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	38
5	Butane, 1-(2-methoxyethoxy)-	132	C7H16O2	013343-98-1	38





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Sample : M4142-05
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Instrument : BNA_M
ClientSampleId : 2087

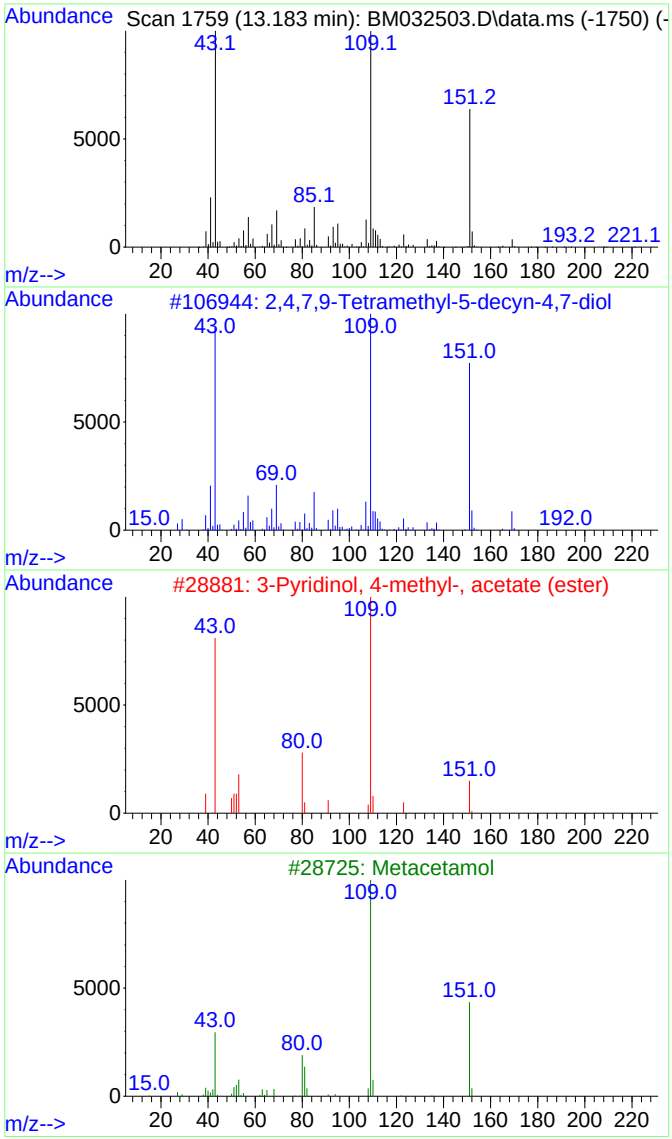
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

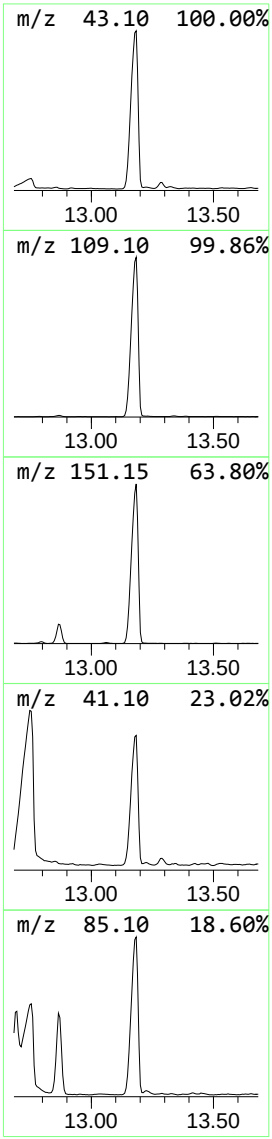
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.183	98.69 ng	15465300	Acenaphthene-d10	14.254

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	53
3	Metacetamol	151	C8H9NO2	000621-42-1	53
4	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	53
5	Ethanone, 1-(1,4-dimethyl-3-cycl...	152	C10H16O	043219-68-7	47





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Sample : M4142-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 2087

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

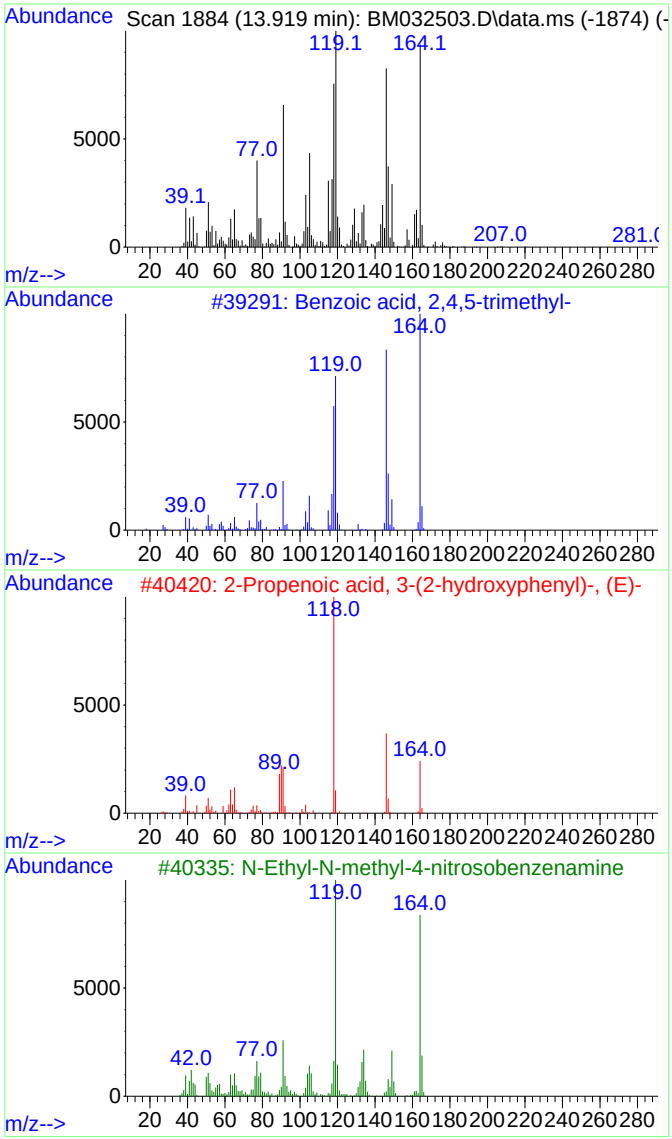
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

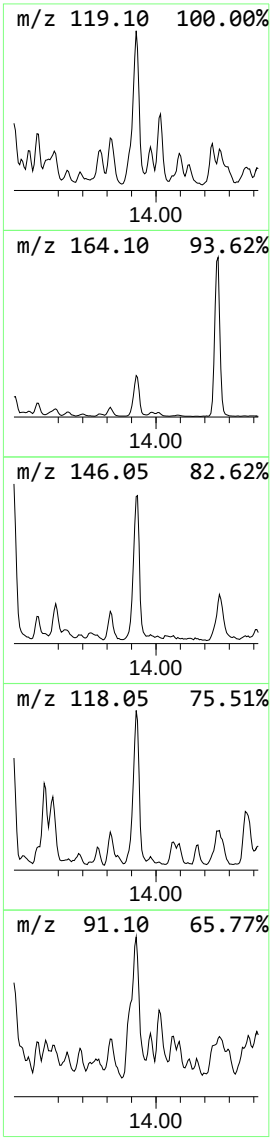
****

Peak Number 15 Benzoic acid, 2,4,5-trimethyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.919	18.59 ng	2913660	Acenaphthene-d10	14.254

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2,4,5-trimethyl-	164	C10H12O2	000528-90-5	93
2	2-Propenoic acid, 3-(2-hydroxyph...	164	C9H8O3	000614-60-8	49
3	N-Ethyl-N-methyl-4-nitrosobenzen...	164	C9H12N2O	036479-98-8	46
4	Benzoic acid, 2,4,6-trimethyl-	164	C10H12O2	000480-63-7	46
5	2,5-Dimethylphenylacetic acid	164	C10H12O2	1000342-65-5	46





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Sample : M4142-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 2087

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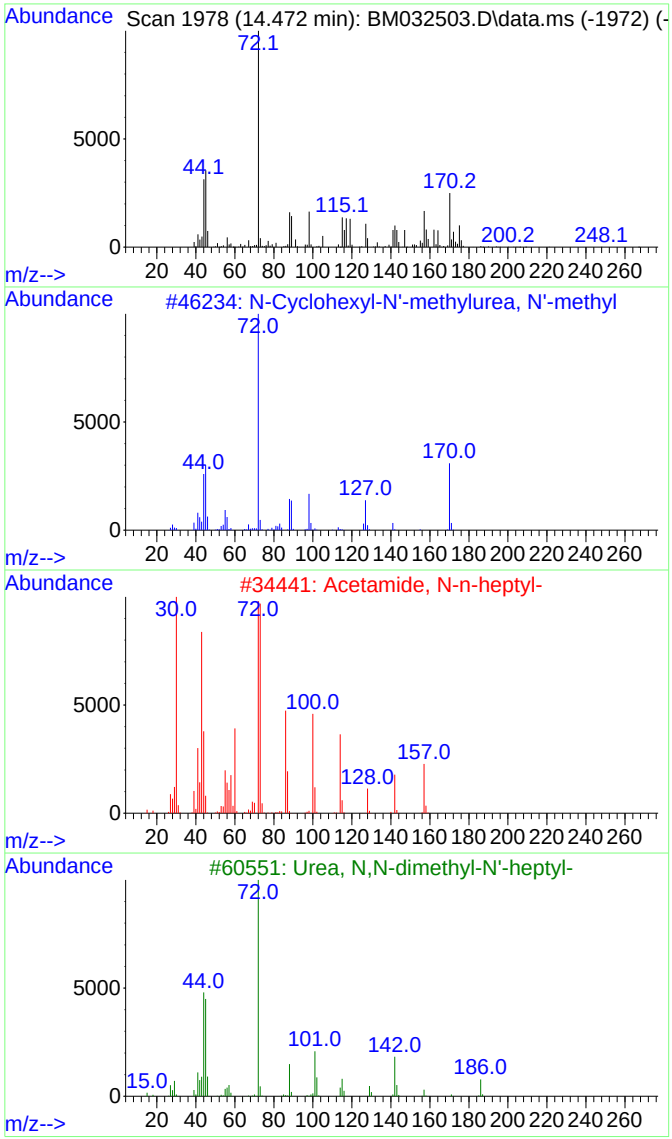
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

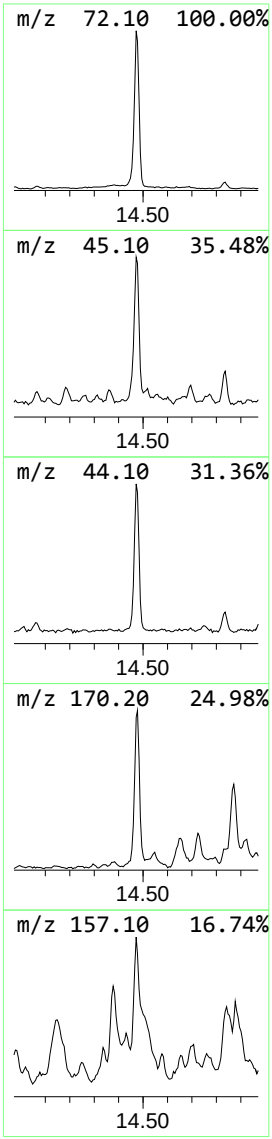
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 16 N-Cyclohexyl-N'-methylurea,... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.472	11.89 ng	1863360	Acenaphthene-d10	14.254

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-Cyclohexyl-N'-methylurea, N'-m...	170	C9H18N2O	031468-12-9	83
2	Acetamide, N-n-heptyl-	157	C9H19NO	1000406-45-2	43
3	Urea, N,N-dimethyl-N'-heptyl-	186	C10H22N2O	1000419-88-5	38
4	Fenuron	164	C9H12N2O	000101-42-8	38
5	2-Propanol, 1-(isopropylamino)-3...	275	C16H21NOS	019343-29-4	35





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Acq On : 13 Oct 2021 19:29
Operator : CG/JU
Sample : M4142-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 2087

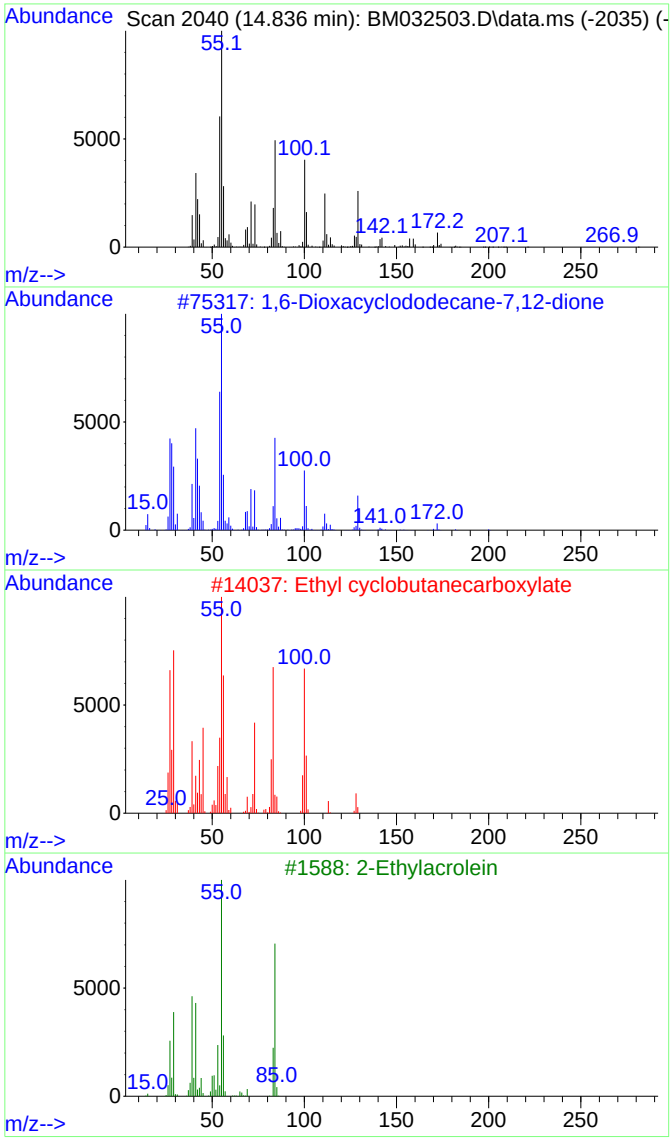
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

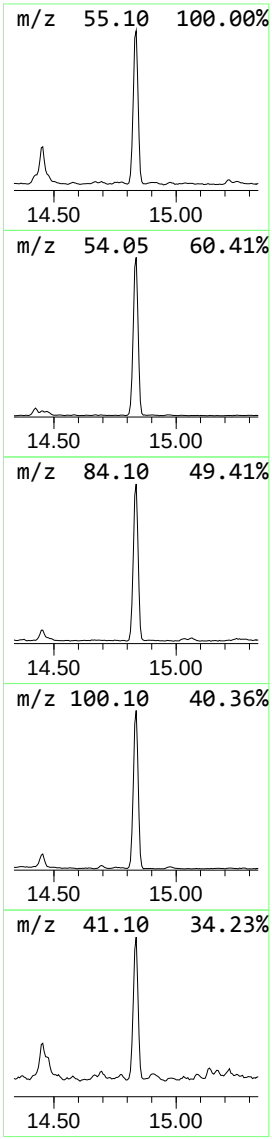
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 17 1,6-Dioxacyclododecane-7,12... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.836	19.06 ng	2986440	Acenaphthene-d10	14.254

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6-Dioxacyclododecane-7,12-dione	200	C10H16O4	000777-95-7	90
2	Ethyl cyclobutanecarboxylate	128	C7H12O2	014924-53-9	12
3	2-Ethylacrolein	84	C5H8O	000922-63-4	11
4	2-Methylcyclopropanecarboxylic acid	100	C5H8O2	029555-02-0	10
5	Pentan-2-yl 2-methylbut-2-enoate	170	C10H18O2	063473-51-8	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101321\
Data File : BM032503.D
Acq On : 13 Oct 2021 19:29
Operator : CG/JU
Sample : M4142-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 2087

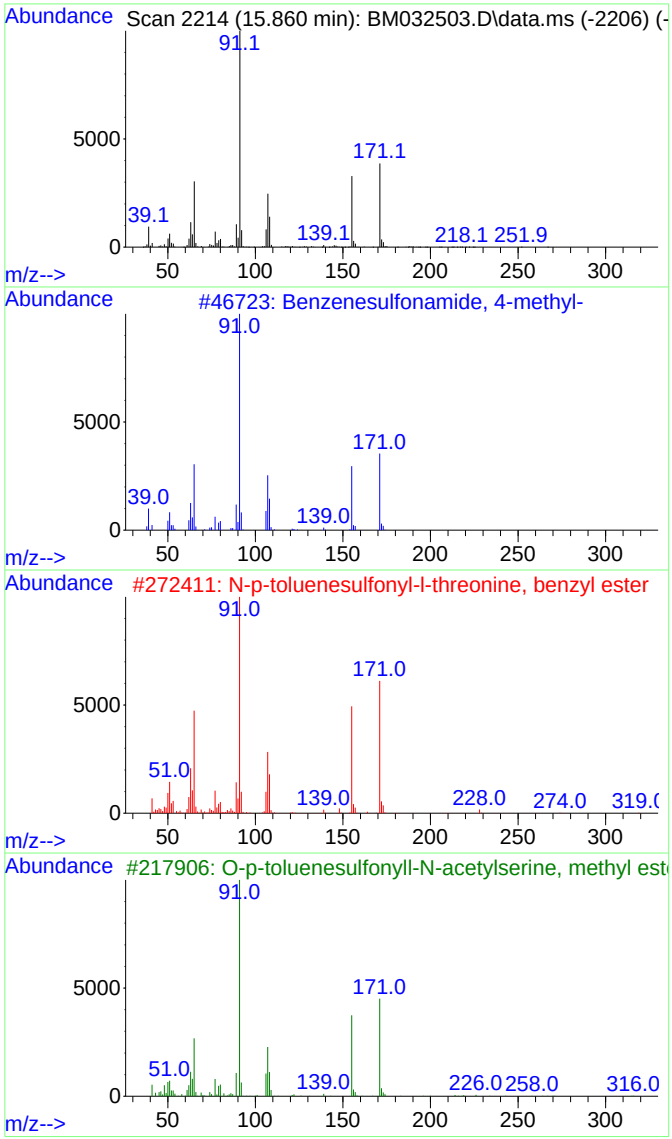
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

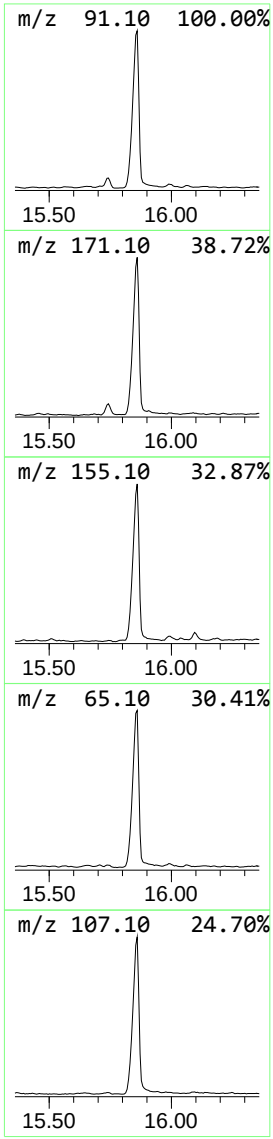
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 18 Benzenesulfonamide, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.860	51.20 ng	5598190	Phenanthrene-d10	16.977

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, 4-methyl-	171	C7H9NO2S	000070-55-3	98
2	N-p-toluenesulfonyl-l-threonine,...	363	C18H21NO5S	1000130-34-4	83
3	O-p-toluenesulfonyll-N-acetylser...	315	C13H17NO6S	1000126-44-8	80
4	Benzenemethanesulfonamide	171	C7H9NO2S	004563-33-1	47
5	Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101321\
Data File : BM032503.D
Acq On : 13 Oct 2021 19:29
Operator : CG/JU
Sample : M4142-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 2087

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

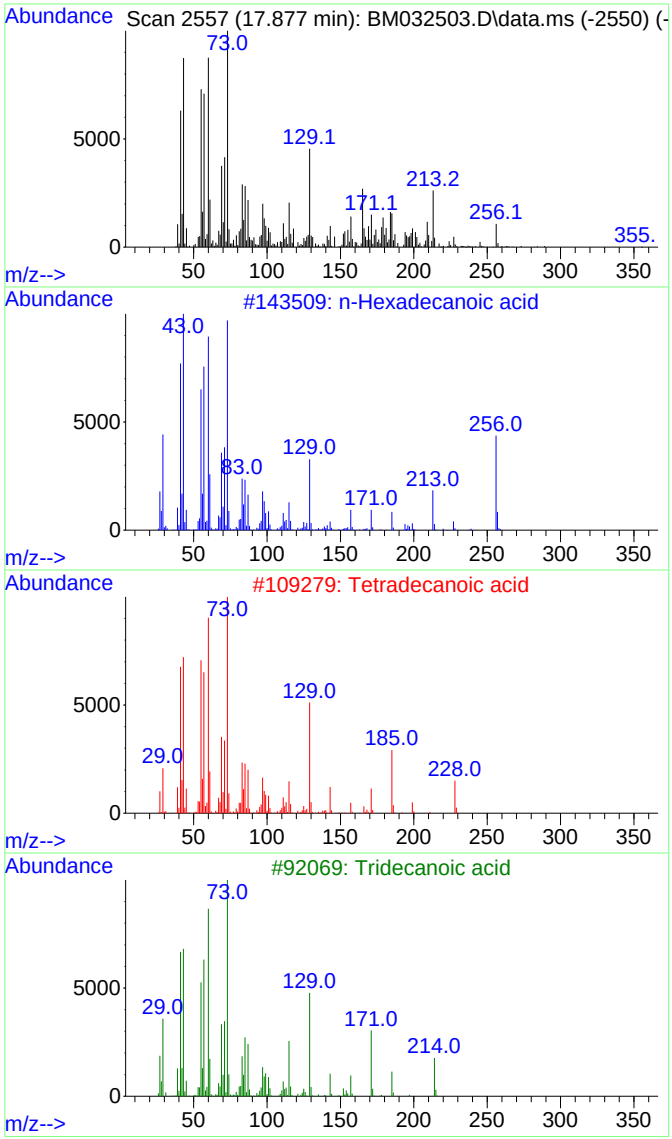
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

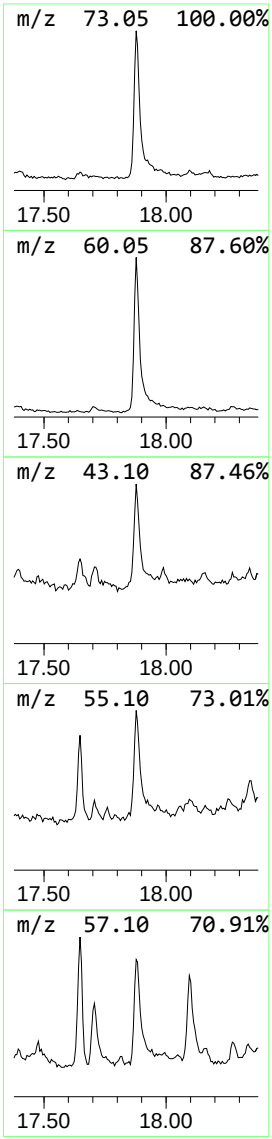
****

Peak Number 19 n-Hexadecanoic acid Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.877	11.93 ng	1304840	Phenanthrene-d10	16.977

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	97
3	Tridecanoic acid	214	C13H26O2	000638-53-9	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5	Octadecanoic acid	284	C18H36O2	000057-11-4	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101321\
Data File : BM032503.D
Acq On : 13 Oct 2021 19:29
Operator : CG/JU
Sample : M4142-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 2087

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

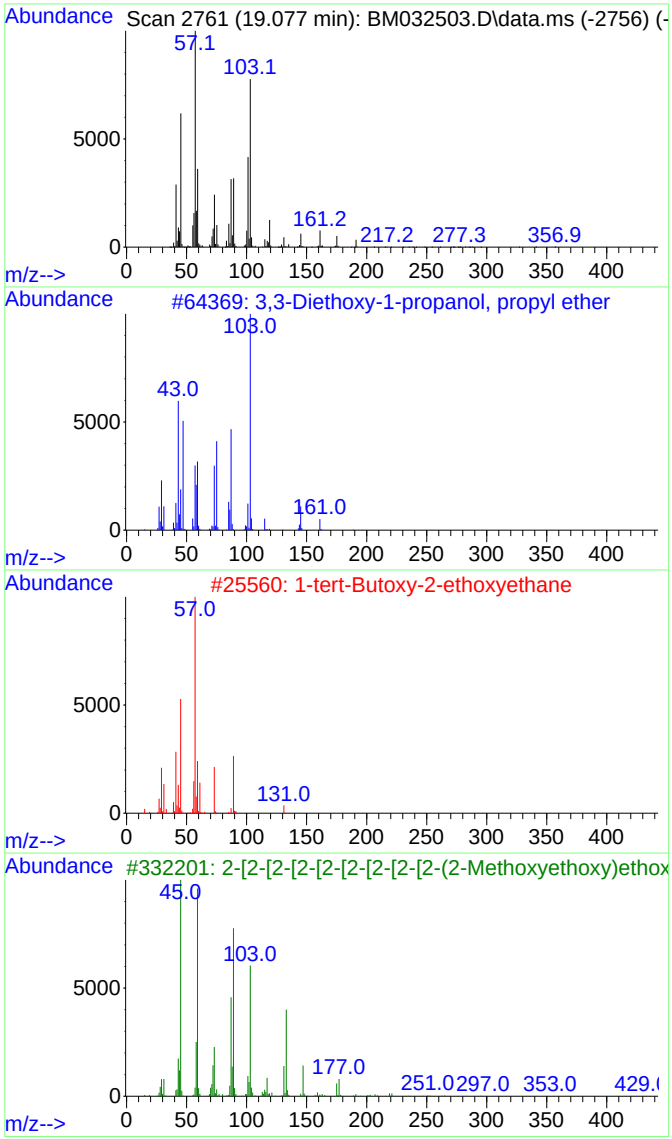
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

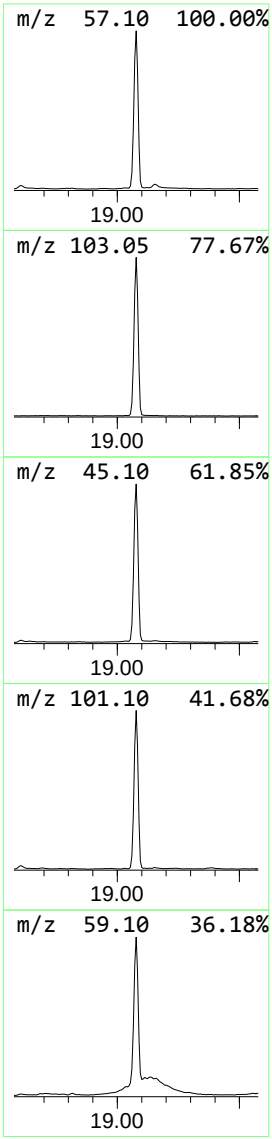
****

Peak Number 20 unknown19.077 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.077	68.49 ng	7356310	Chrysene-d12	21.148

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,3-Diethoxy-1-propanol, propyl ...	190	C10H22O3	1000395-37-1	43
2	1-tert-Butoxy-2-ethoxyethane	146	C8H18O2	051422-54-9	27
3	2-[2-[2-[2-[2-[2-[2-[2-(2-Met...	472	C21H44O11	027425-92-9	25
4	Propane, 1,1,3,3-tetraethoxy-	220	C11H24O4	000122-31-6	22
5	Butane, 1,1'-[ethylidenebis(oxy)...	174	C10H22O2	000871-22-7	22





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101321\
Data File : BM032503.D
Acq On : 13 Oct 2021 19:29
Operator : CG/JU
Sample : M4142-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 2087

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.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
unknown3.731	3.731	11.5	ng	721924	1	7.601	1251890	20.0
Butanoic acid, ...	6.143	18.0	ng	1124980	1	7.601	1251890	20.0
1-Hexanol, 2-et...	7.684	22.0	ng	1377210	1	7.601	1251890	20.0
Butoxyacetic acid	8.707	196.7	ng	12313600	1	7.601	1251890	20.0
Hexanoic acid, ...	9.060	36.1	ng	3046860	2	10.389	1686840	20.0
unknown9.142	9.142	10.9	ng	916828	2	10.389	1686840	20.0
Ethanol, 2-(2-b...	10.178	14.2	ng	1196570	2	10.389	1686840	20.0
2-Propanol, 1,1...	10.937	28.6	ng	2410560	2	10.389	1686840	20.0
2-Propanol, 1-(...	10.995	29.0	ng	2444010	2	10.389	1686840	20.0
Benzothiazole	11.031	22.4	ng	1886980	2	10.389	1686840	20.0
Benzoic acid, 4...	11.460	40.7	ng	3433910	2	10.389	1686840	20.0
1H-Inden-1-one,...	11.766	14.5	ng	1223490	2	10.389	1686840	20.0
2-(2-Butoxyetho...	12.748	88.6	ng	13890500	3	14.254	3133990	20.0
2,4,7,9-Tetrame...	13.183	98.7	ng	15465300	3	14.254	3133990	20.0
Benzoic acid, 2...	13.919	18.6	ng	2913660	3	14.254	3133990	20.0
N-Cyclohexyl-N'...	14.472	11.9	ng	1863360	3	14.254	3133990	20.0
1,6-Dioxacyclod...	14.836	19.1	ng	2986440	3	14.254	3133990	20.0
Benzenesulfonam...	15.860	51.2	ng	5598190	4	16.977	2186750	20.0
n-Hexadecanoic ...	17.877	11.9	ng	1304840	4	16.977	2186750	20.0
unknown19.077	19.077	68.5	ng	7356310	5	21.148	2148130	20.0