LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
Data File : BF137342.D
Acq On : 08 Feb 2024 17:21
Operator : CG\JU
Sample : P1342-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323P-GW-20240131-1

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137342.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.116	166	175	180	rBV	352302	644856	18.22%	1.468%
2	3.646	256	265	273	rVB3	71132	134963	3.81%	0.307%
3	4.128	340	347	352	rVB	54094	74295	2.10%	0.169%
4	4.557	412	420	427	rBV	64691	87590	2.48%	0.199%
5	5.069	503	507	513	rVV4	57815	107128	3.03%	0.244%
6	5.134	513	518	527	rVB3	50254	71807	2.03%	0.163%
7	5.410	562	565	574	rBV	1144891	1133588	32.04%	2.580%
8	6.116	679	685	688	rBV3	82715	105542	2.98%	0.240%
9	6.216	698	702	706	rVB3	58356	71329	2.02%	0.162%
10	6.298	710	716	720	rBV2	74016	85495	2.42%	0.195%
11	6.381	727	730	733	rBV3	69009	76848	2.17%	0.175%
12	6.416	733	736	745	rVV	748719	834267	23.58%	1.899%
13	6.710	782	786	789	rBV3	63598	78082	2.21%	0.178%
14	6.787	794	799	802	rBV	644322	681023	19.25%	1.550%
15	6.816	802	804	807	rVV	240808	215264	6.08%	0.490%
16	6.845	807	809	814	rVB	72930	69529	1.97%	0.158%
17	6.928	821	823	826	rBV	174066	149720	4.23%	0.341%
18	6.992	828	834	835	rBV4	115773	187528	5.30%	0.427%
19	7.028	835	840	842	rBV2	109690	167840	4.74%	0.382%
20	7.110	850	854	863	rBV5	191149	287221	8.12%	0.654%
21	7.187	863	867	870	rVV2	61187	88782	2.51%	0.202%
22	7.257	874	879	882	rVV2	122778	167704	4.74%	0.382%
23	7.292	882	885	886	rVV	83108	78058	2.21%	0.178%
24	7.345	886	894	899	rVV	1926745	2690693	76.04%	6.123%
25	7.392	899	902	905	rVV2	346206	438229	12.39%	0.997%
26	7.422	905	907	912	rVV5	93401	159727	4.51%	0.364%
27	7.463	912	914	917	rVV2	125650	128096	3.62%	0.292%
28	7.510	917	922	926	rVV3	93188	131208	3.71%	0.299%
29	7.551	926	929	932	rVB3	148156	130971	3.70%	0.298%
30	7.604	935	938	939	rVV2	177582	198800	5.62%	0.452%
31	7.634	939	943	945	rVV2	380839	561122	15.86%	1.277%
32	7.675	947	950	953	rVV2	202201	236964	6.70%	0.539%
33	7.704	953	955	959	rVV4	76191	87487	2.47%	0.199%
34	7.751	961	963	967	rVB3	82406	77804	2.20%	0.177%
35	7.804	967	972	976	rBV5	107962	192462	5.44%	0.438%
36	7.898	985	988	991	rBV3	108277	134282	3.80%	0.306%

LSC Area Percent Report

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Operator : CG\JU
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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323P-GW-20240131-1

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	7.939	991	995	998	rVV4	203230	257246	7.27%	0.585%
38	7.998	1002	1005	1010	rVV3	175371	254676	7.20%	0.580%
39	8.063	1012	1016	1018	rVV	891497	782819	22.12%	1.782%
40	8.122	1022	1026	1030	rVB5	68202	130476	3.69%	0.297%
41	8.186	1032	1037	1040	rBV	303807	346726	9.80%	0.789%
42	8.239	1040	1046	1050	rVV6	133140	207119	5.85%	0.471%
43	8.275	1050	1052	1053	rVV2	71104	70762	2.00%	0.161%
44	8.292	1053	1055	1057	rVV2	236796	300151	8.48%	0.683%
45	8.333	1058	1062	1066	rVV	2385936	2709805	76.58%	6.167%
46	8.369	1066	1068	1071	rVV3	194824	241775	6.83%	0.550%
47	8.433	1074	1079	1083	rVV	216283	335283	9.48%	0.763%
48	8.469	1083	1085	1088	rVV4	141209	177608	5.02%	0.404%
49	8.498	1088	1090	1096	rVV3	225684	328389	9.28%	0.747%
50	8.551	1097	1099	1103	rVB4	115403	103283	2.92%	0.235%
51	8.592	1103	1106	1109	rBV2	512398	541033	15.29%	1.231%
52	8.628	1109	1112	1113	rVV2	155034	160953	4.55%	0.366%
53	8.669	1113	1119	1121	rVV	3281275	3538314	100.00%	8.052%
54	8.692	1121	1123	1127	rVV4	146104	191568	5.41%	0.436%
55	8.739	1127	1131	1133	rVV3	252881	343677	9.71%	0.782%
56	8.786	1133	1139	1140	rVV4	400464	747231	21.12%	1.701%
57	8.804	1140	1142	1145	rVV	744729	693730	19.61%	1.579%
58	8.845	1147	1149	1151	rVV	142979	137974	3.90%	0.314%
59	8.880	1151	1155	1157	rVV	1099407	1090446	30.82%	2.482%
60	8.898	1157	1158	1160	rVV3	351688	269923	7.63%	0.614%
61	8.922	1160	1162	1165	rVV2	501793	543956	15.37%	1.238%
62	8.951	1165	1167	1174	rVB3	314427	441969	12.49%	1.006%
63	9.010	1174	1177	1180	rBV2	278915	286141	8.09%	0.651%
64	9.045	1180	1183	1184	rBV	230729	215940	6.10%	0.491%
65	9.069	1184	1187	1190	rVV3	403216	394577	11.15%	0.898%
66	9.110	1191	1194	1196	rVV	492633	444182	12.55%	1.011%
67	9.145	1196	1200	1203	rVB	3706334	3148479	88.98%	7.165%
68	9.175	1203	1205	1209	rBV3	117202	144072	4.07%	0.328%
69	9.222	1209	1213	1218	rBV4	180614	297326	8.40%	0.677%
70	9.304	1224	1227	1231	rVB2	380416	341148	9.64%	0.776%
71	9.351	1231	1235	1236	rBV2	173336	201712	5.70%	0.459%
72	9.386	1236	1241	1243	rVV2	412119	494305	13.97%	1.125%
73	9.410	1243	1245	1250	rVB2	737308	889985	25.15%	2.025%
74	9.457	1250	1253	1258	rBV2	271878	369348	10.44%	0.841%
75	9.528	1263	1265	1268	rVB2	173728	173907	4.91%	0.396%
76	9.586	1268	1275	1279	rBV	709077	750219	21.20%	1.707%

LSC Area Percent Report

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Sample : P1342-07
Misc :
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Instrument :
BNA_F
ClientSampleId :
MR-323P-GW-20240131-1

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
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Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	9.704	1293	1295	1298	rBV	153315	118230	3.34%	0.269%
78	9.757	1300	1304	1308	rVV2	367963	454997	12.86%	1.035%
79	9.792	1308	1310	1312	rVV2	226713	215428	6.09%	0.490%
80	9.822	1312	1315	1321	rVV	893113	890416	25.16%	2.026%
81	9.880	1321	1325	1327	rVV5	100422	138331	3.91%	0.315%
82	9.916	1327	1331	1335	rVV4	189952	291059	8.23%	0.662%
83	9.951	1335	1337	1339	rVV	118636	100021	2.83%	0.228%
84	9.975	1339	1341	1348	rVB3	263397	343880	9.72%	0.783%
85	10.104	1358	1363	1366	rBV5	75620	124301	3.51%	0.283%
86	10.175	1371	1375	1378	rVV3	216928	267777	7.57%	0.609%
87	10.210	1378	1381	1385	rVV4	171877	217855	6.16%	0.496%
88	10.245	1385	1387	1391	rVV4	126453	169206	4.78%	0.385%
89	10.286	1391	1394	1396	rVV2	101839	98619	2.79%	0.224%
90	10.433	1417	1419	1426	rVB2	188856	192780	5.45%	0.439%
91	10.610	1445	1449	1456	rBV	1862373	1771672	50.07%	4.032%
92	10.739	1467	1471	1479	rVB8	77408	137685	3.89%	0.313%
93	11.186	1544	1547	1549	rBV	103618	75493	2.13%	0.172%
94	11.310	1564	1568	1572	rVB	792865	641139	18.12%	1.459%
95	11.851	1657	1660	1669	rVB2	247333	263139	7.44%	0.599%
96	12.645	1792	1795	1799	rBV	68419	72309	2.04%	0.165%
97	12.910	1836	1840	1843	rBV	2594565	2266437	64.05%	5.158%
98	13.827	1993	1996	2003	rVB	91786	103465	2.92%	0.235%
99	13.963	2016	2019	2026	rVB	556064	508458	14.37%	1.157%
100	15.445	2266	2271	2277	rBV	484094	613417	17.34%	1.396%

Sum of corrected areas: 43940651

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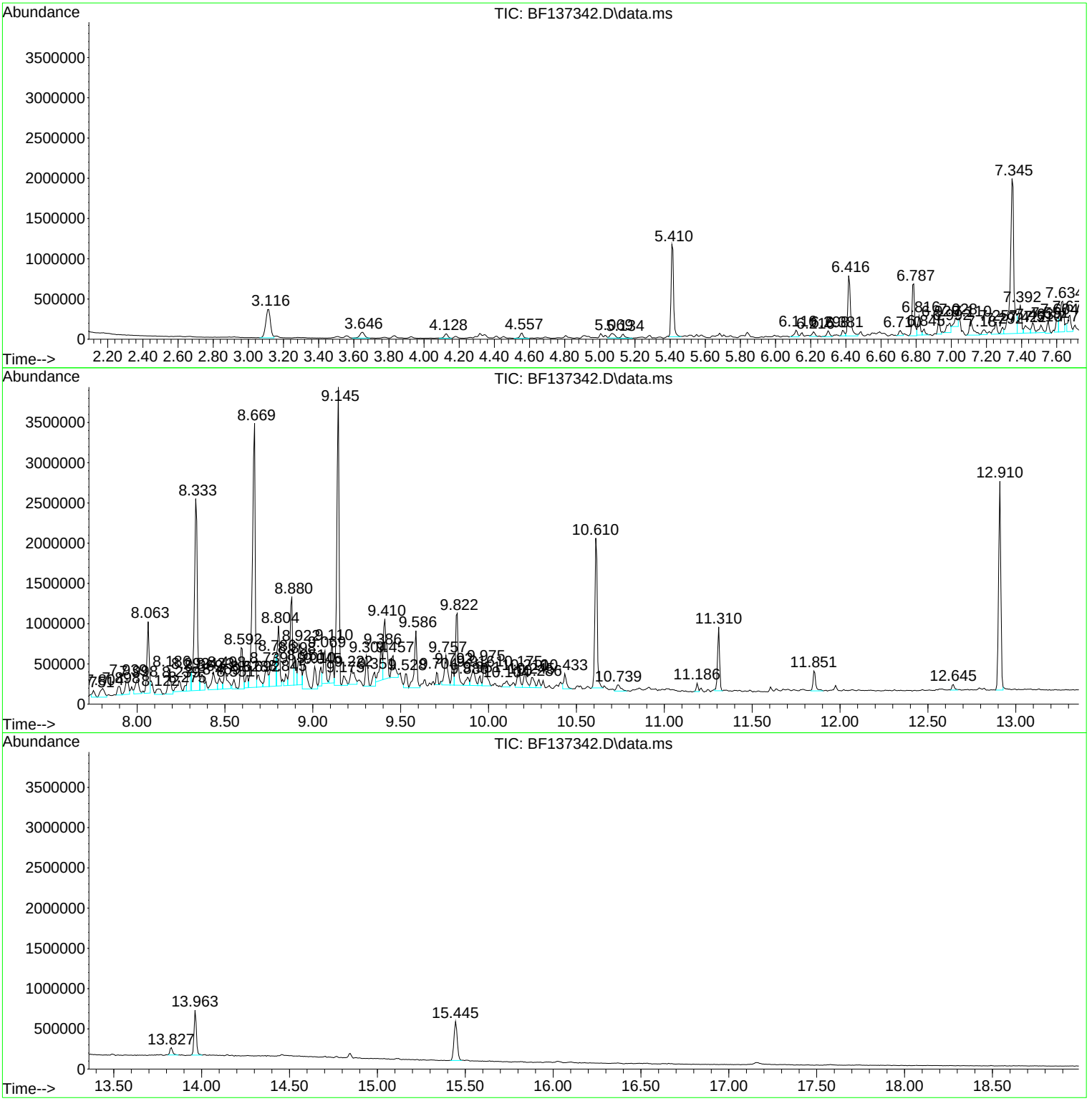
Instrument :
BNA_F
ClientSampleId :
MR-323P-GW-20240131-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
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Instrument :
BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

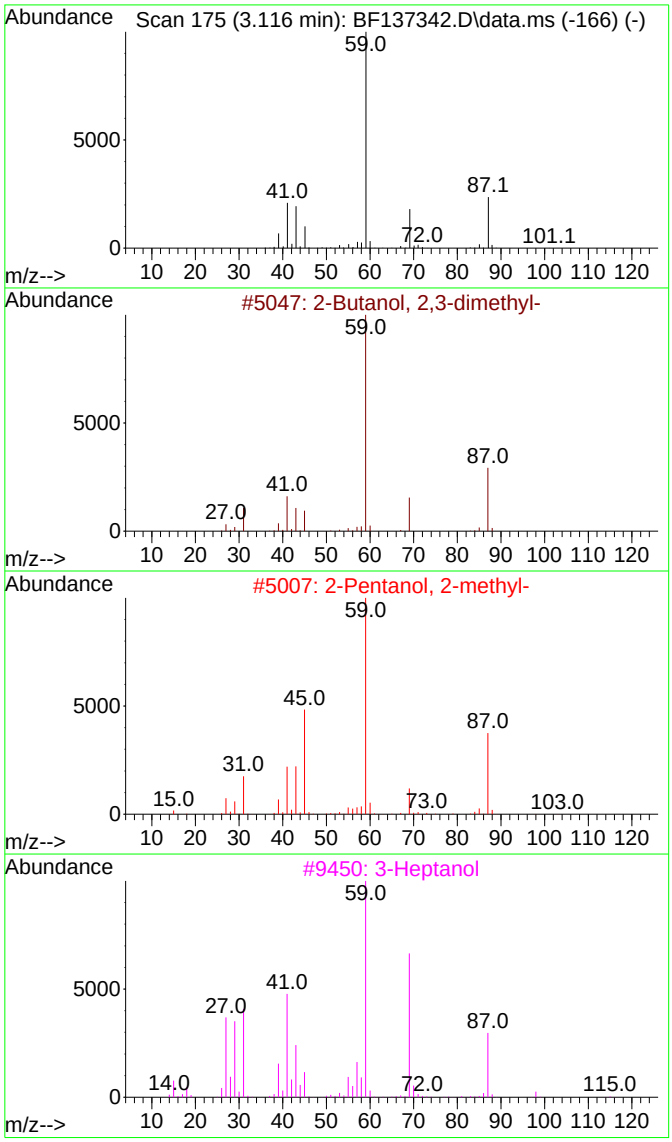
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

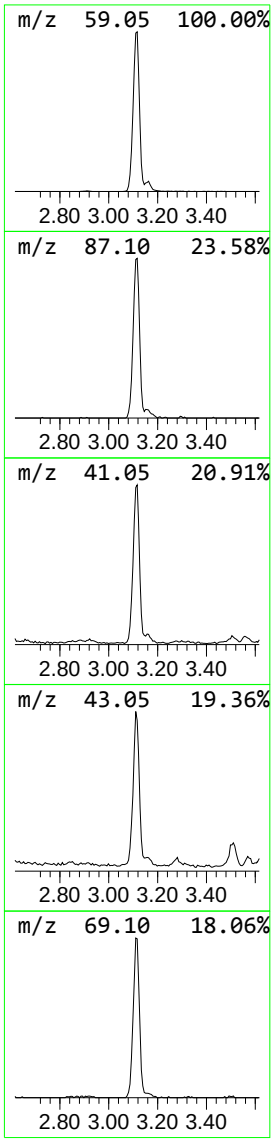
****

Peak Number 1 2-Butanol, 2,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.116	18.94 ng	644856	1,4-Dichlorobenzene-d4	6.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	83
2	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	56
3	3-Heptanol	116	C7H16O	000589-82-2	40
4	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	39
5	2-Decanol, methyl ether	172	C11H24O	1000333-83-9	33





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MR-323P-GW-20240131-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

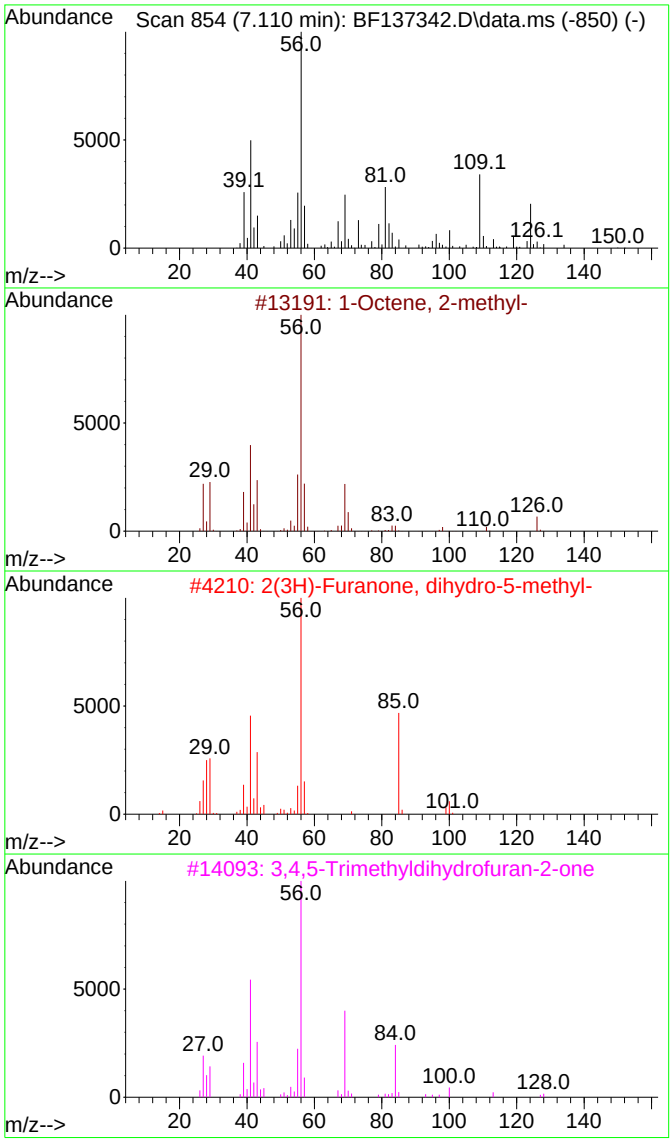
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

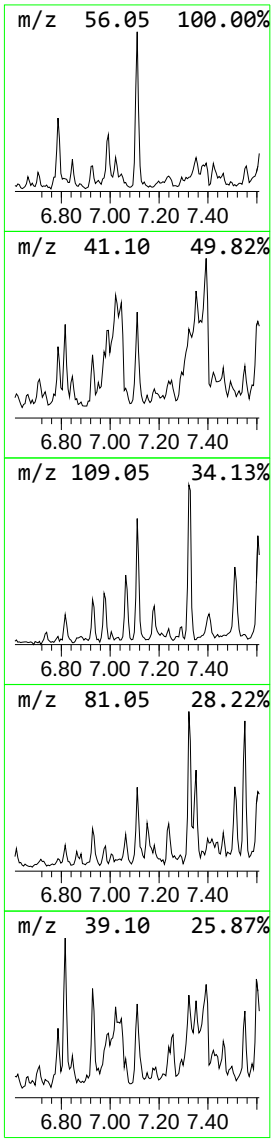
****

Peak Number 2 unknown7.110 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.110	8.43 ng	287221	1,4-Dichlorobenzene-d4	6.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octene, 2-methyl-	126	C9H18	004588-18-5	38
2	2(3H)-Furanone, dihydro-5-methyl-	100	C5H8O2	000108-29-2	38
3	3,4,5-Trimethyldihydrofuran-2-one	128	C7H12O2	1000194-05-2	38
4	1-Heptene, 2-methyl-	112	C8H16	015870-10-7	38
5	Furan, tetrahydro-2,5-dimethyl-,...	100	C6H12O	002144-41-4	38





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

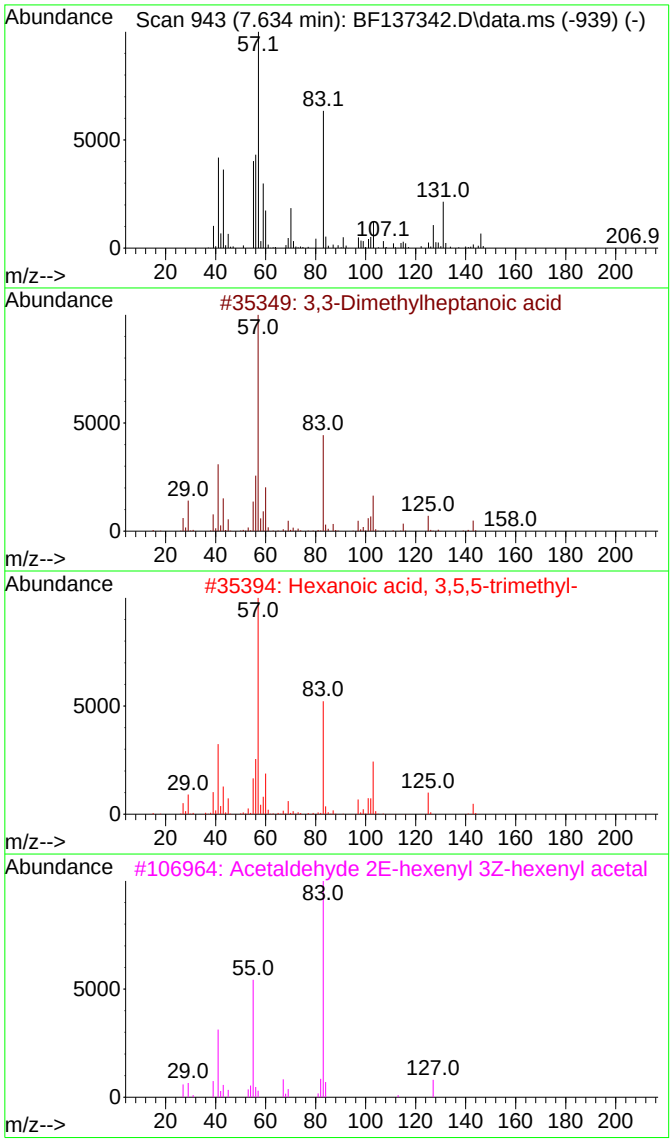
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

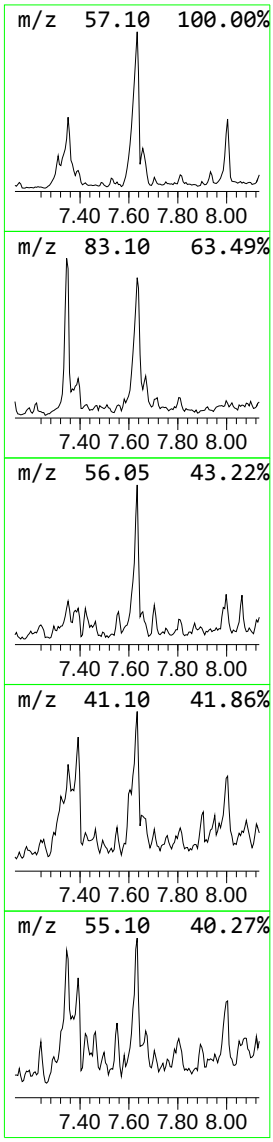
****

Peak Number 3 unknown7.634 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.634	14.34 ng	561122	Naphthalene-d8	8.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,3-Dimethylheptanoic acid	158	C9H18O2	067061-30-7	32
2	Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	32
3	Acetaldehyde 2E-hexenyl 3Z-hexen...	226	C14H26O2	1000431-45-5	10
4	Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	10
5	Acetamide, N-2-propenyl-	99	C5H9NO	000692-33-1	10





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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323P-GW-20240131-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

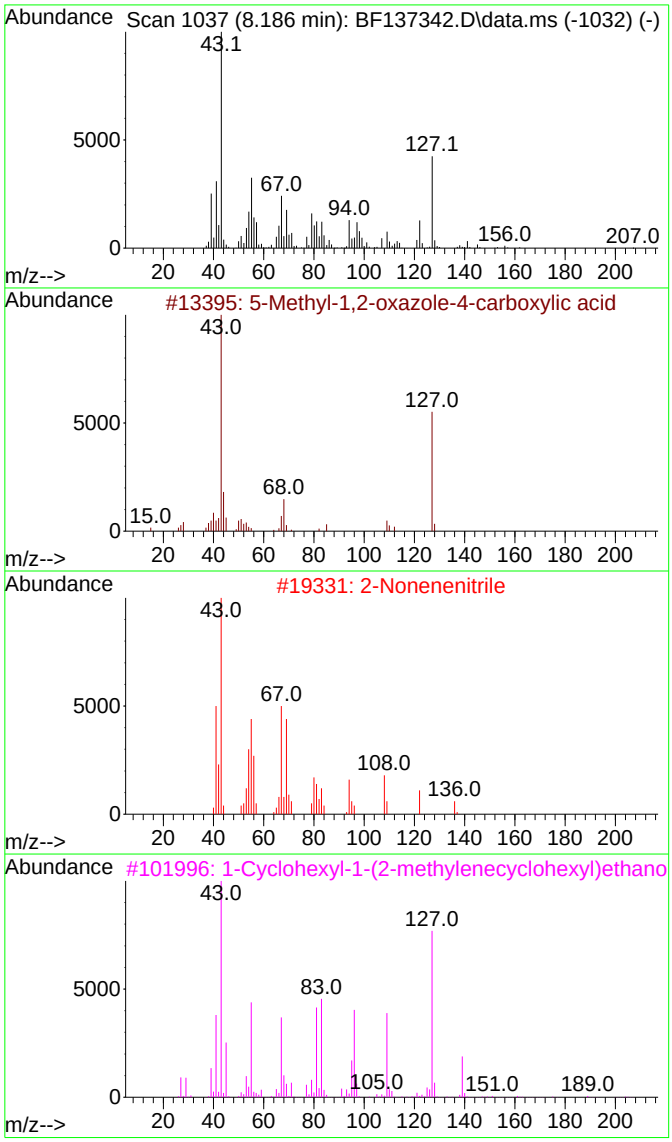
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

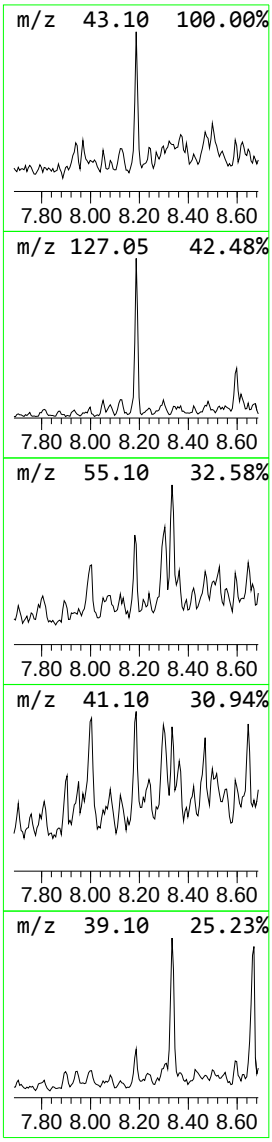
****

Peak Number 4 unknown8.186 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.186	8.86 ng	346726	Naphthalene-d8	8.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Methyl-1,2-oxazole-4-carboxyli...	127	C5H5NO3	042831-50-5	27
2	2-Nonenenitrile	137	C9H15N	029127-83-1	25
3	1-Cyclohexyl-1-(2-methylenecyclo...	222	C15H26O	1000191-92-7	25
4	Cyclohexanepropanol, 2-acetoxy-	200	C11H20O3	1000197-25-8	25
5	4-Isopropyl-5-methylhex-2-yne-1,...	170	C10H18O2	070372-89-3	25





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Data File : BF137342.D
Acq On : 08 Feb 2024 17:21
Operator : CG\JU
Sample : P1342-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323P-GW-20240131-1

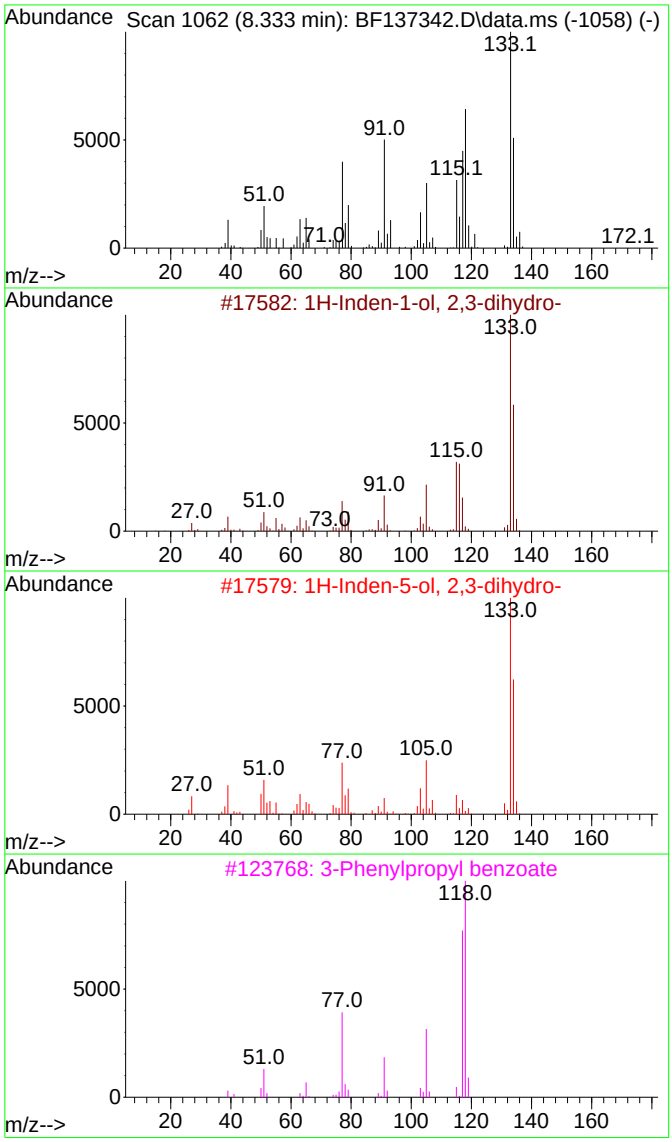
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

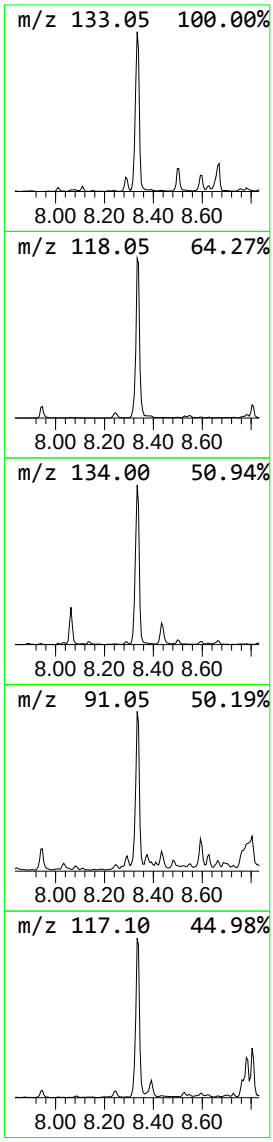
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1H-Inden-1-ol, 2,3-dihydro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.333	69.23 ng	2709810	Naphthalene-d8	8.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Inden-1-ol, 2,3-dihydro-	134	C9H10O	006351-10-6	58
2	1H-Inden-5-ol, 2,3-dihydro-	134	C9H10O	001470-94-6	45
3	3-Phenylpropyl benzoate	240	C16H16O2	060045-26-3	38
4	Benzenecarboximidamide, 4-methyl-	134	C8H10N2	018465-11-7	35
5	Pyrazine, 2-methyl-6-(1-propenyl...	134	C8H10N2	055138-67-5	30





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Sample : P1342-07
Misc :
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Instrument :
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ClientSampleId :
MR-323P-GW-20240131-1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

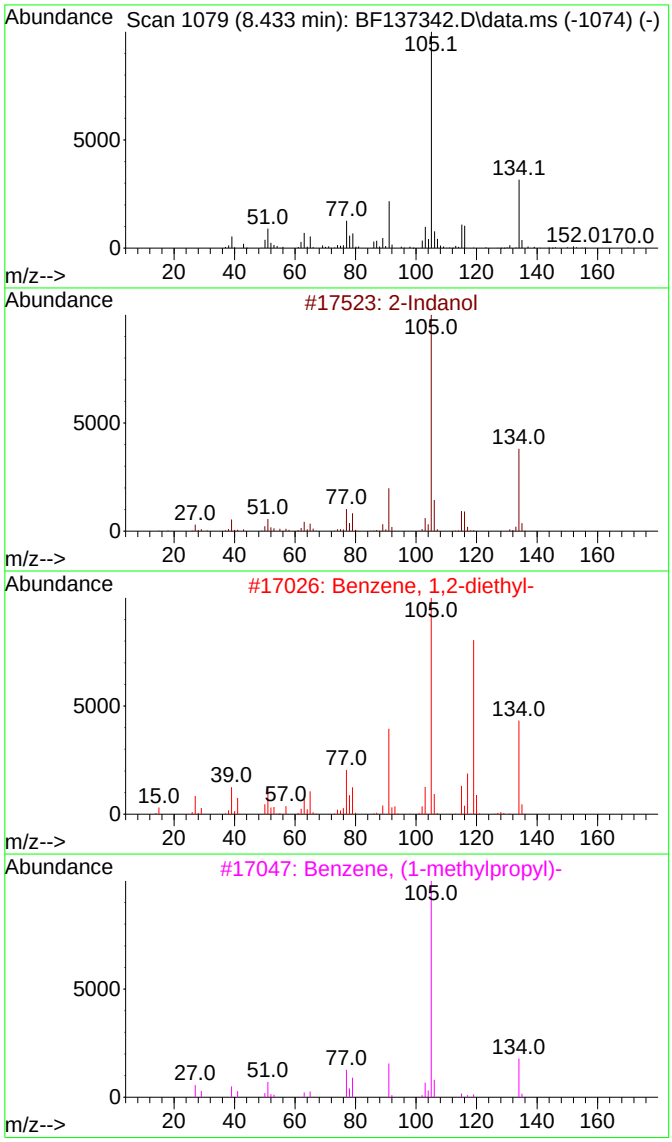
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

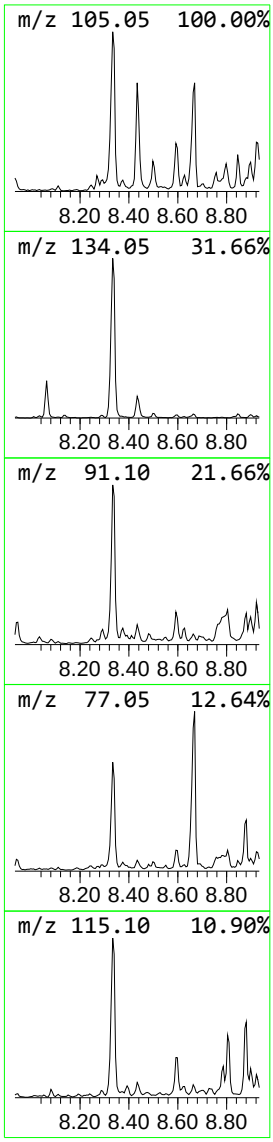
****

Peak Number 6 2-Indanol Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.433	8.57 ng	335283	Naphthalene-d8	8.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Indanol	134	C9H10O	004254-29-9	87
2	Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	70
3	Benzene, (1-methylpropyl)-	134	C10H14	000135-98-8	58
4	Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	52
5	Oxirane, 2-methyl-2-phenyl-	134	C9H10O	002085-88-3	50





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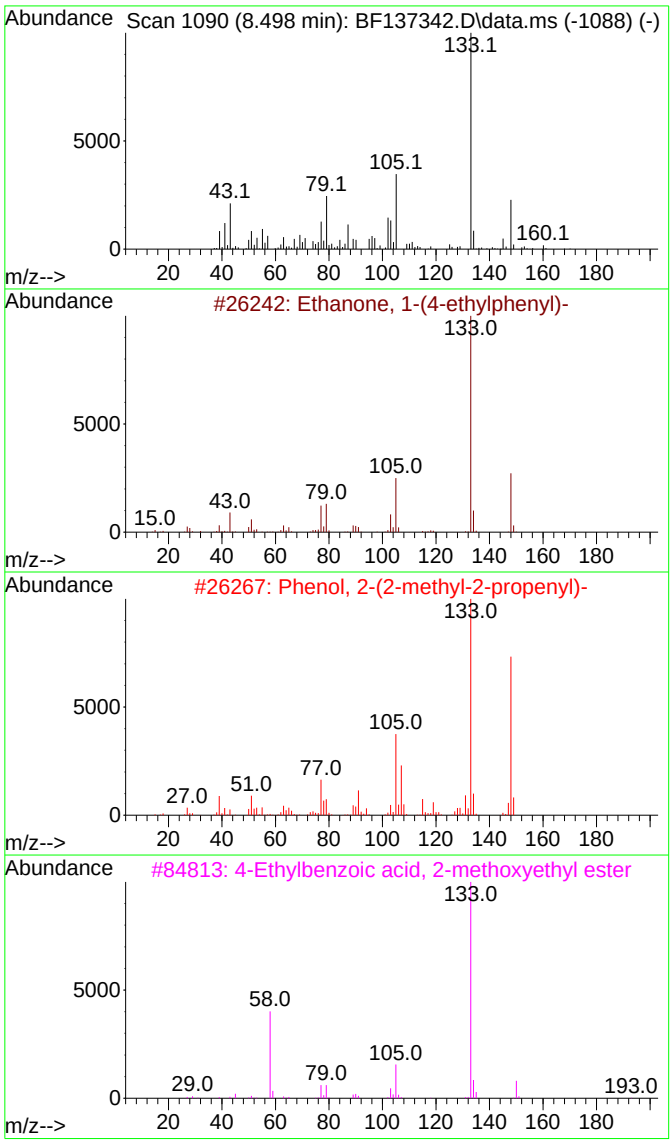
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

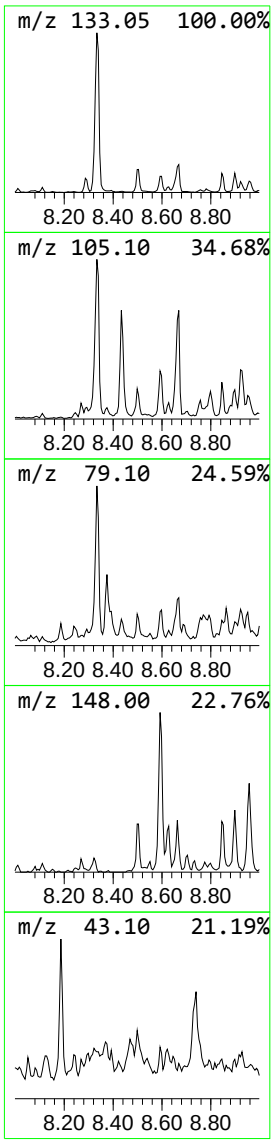
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Ethanone, 1-(4-ethylphenyl)- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.498	8.39 ng	328389	Naphthalene-d8	8.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanone, 1-(4-ethylphenyl)-	148	C10H12O	000937-30-4	81
2	Phenol, 2-(2-methyl-2-propenyl)-	148	C10H12O	020944-88-1	52
3	4-Ethylbenzoic acid, 2-methoxyet...	208	C12H16O3	1000331-30-6	50
4	Benzene, 1-(1,1-dimethylethyl)-3...	148	C11H16	001075-38-3	50
5	4-tert-Butyltoluene	148	C11H16	000098-51-1	50





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

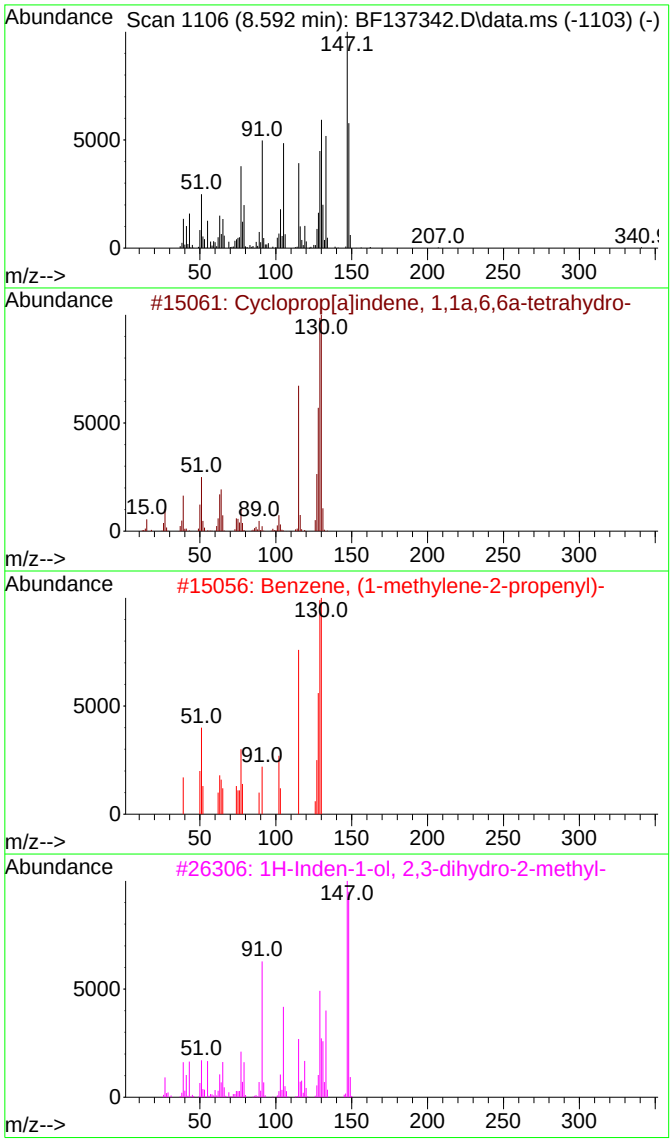
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

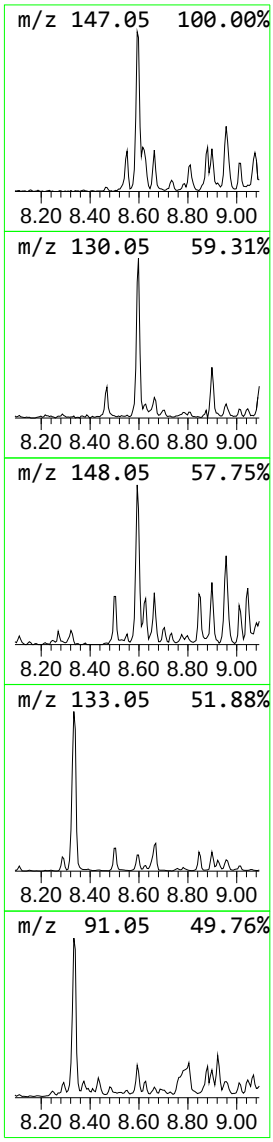
****

Peak Number 8 unknown8.592 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.592	13.82 ng	541033	Naphthalene-d8	8.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	38
2	Benzene, (1-methylene-2-propenyl)-	130	C10H10	002288-18-8	38
3	1H-Inden-1-ol, 2,3-dihydro-2-met...	148	C10H12O	017496-18-3	35
4	1H-Indene, 1-methyl-	130	C10H10	000767-59-9	30
5	Benzene, 1,3-butadienyl-	130	C10H10	001515-78-2	25





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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MR-323P-GW-20240131-1

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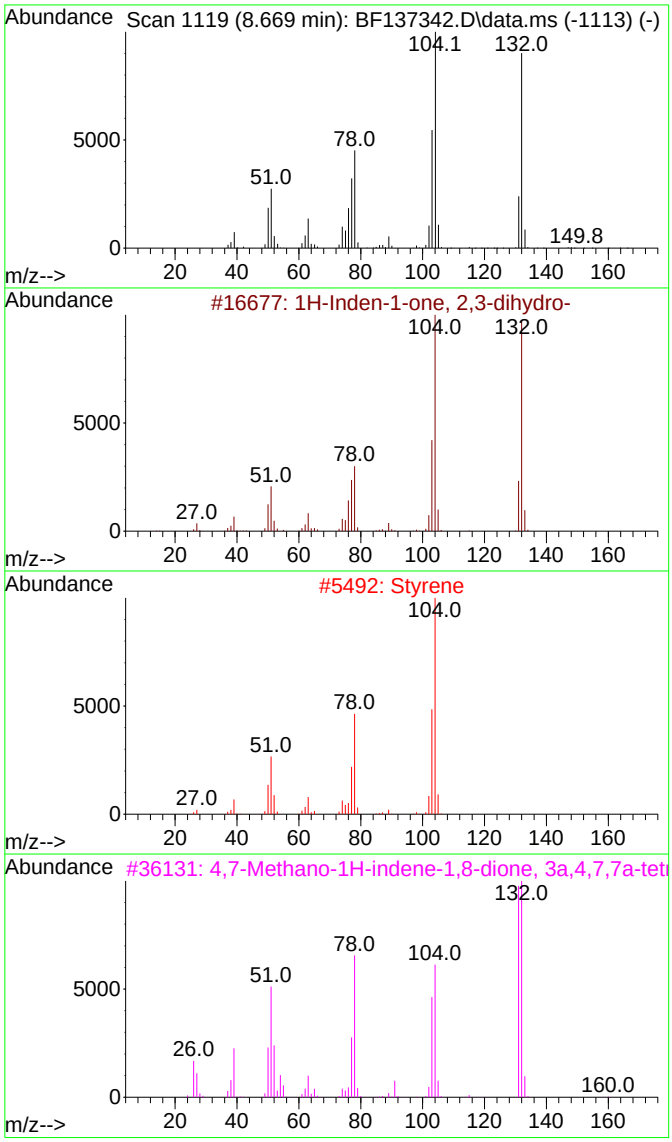
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

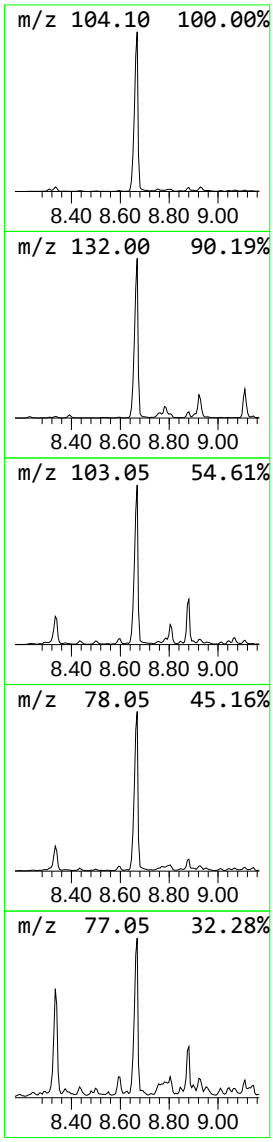
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1H-Inden-1-one, 2,3-dihydro- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.669	90.40 ng	3538310	Naphthalene-d8	8.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Inden-1-one, 2,3-dihydro-	132	C9H8O	000083-33-0	96
2	Styrene	104	C8H8	000100-42-5	91
3	4,7-Methano-1H-indene-1,8-dione,...	160	C10H8O2	000826-65-3	81
4	1,3,5,7-Cyclooctatetraene	104	C8H8	000629-20-9	64
5	Bicyclo[4.2.0]octa-1,3,5-triene	104	C8H8	000694-87-1	64





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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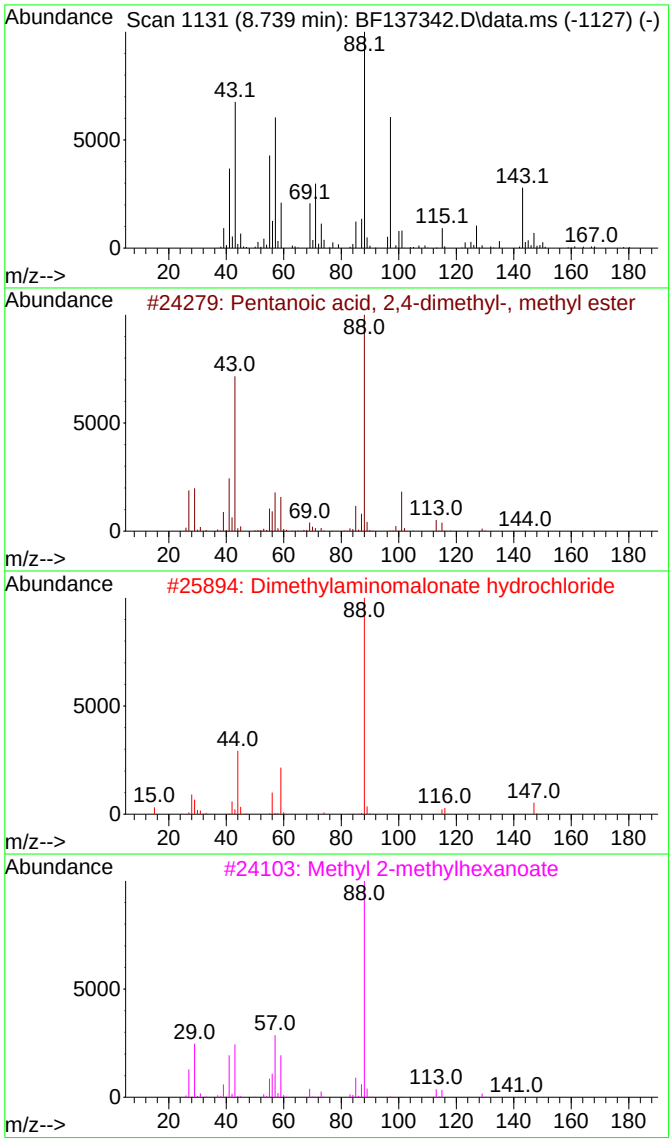
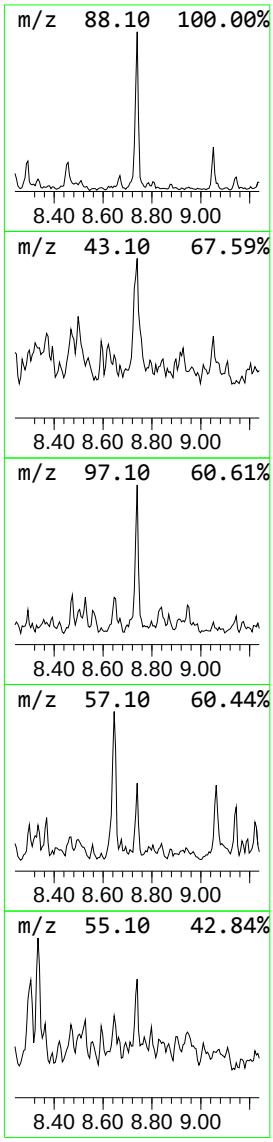
Peak Number 10 unknown8.739 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.739	8.78 ng	343677	Naphthalene-d8	8.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanoic acid, 2,4-dimethyl-, m...	144	C8H16O2	071672-33-8	38
2	Dimethylaminomalonate hydrochloride	147	C5H9NO4	016115-80-3	38
3	Methyl 2-methylhexanoate	144	C8H16O2	002177-81-3	38
4	Hexanoic acid, 2,4-dimethyl-, me...	158	C9H18O2	014251-45-7	37
5	Glycine, N-(methoxycarbonyl)-, m...	147	C5H9NO4	070288-73-2	35





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

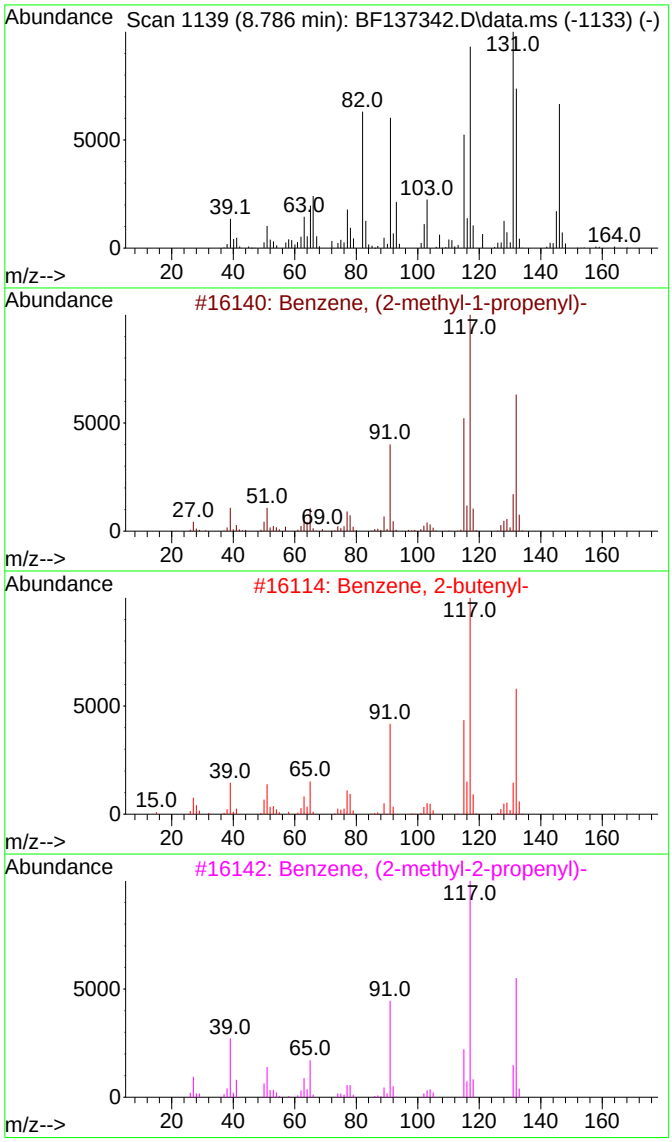
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

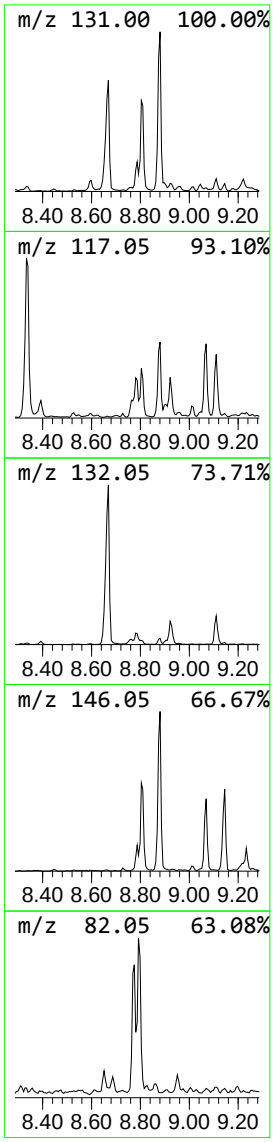
****

Peak Number 11 unknown8.786 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.786	19.09 ng	747231	Naphthalene-d8	8.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	46
2	Benzene, 2-butenyl-	132	C10H12	001560-06-1	46
3	Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	42
4	2,4-Dimethylstyrene	132	C10H12	002234-20-0	41
5	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	41





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Sample : P1342-07
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Instrument :
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ClientSampleId :
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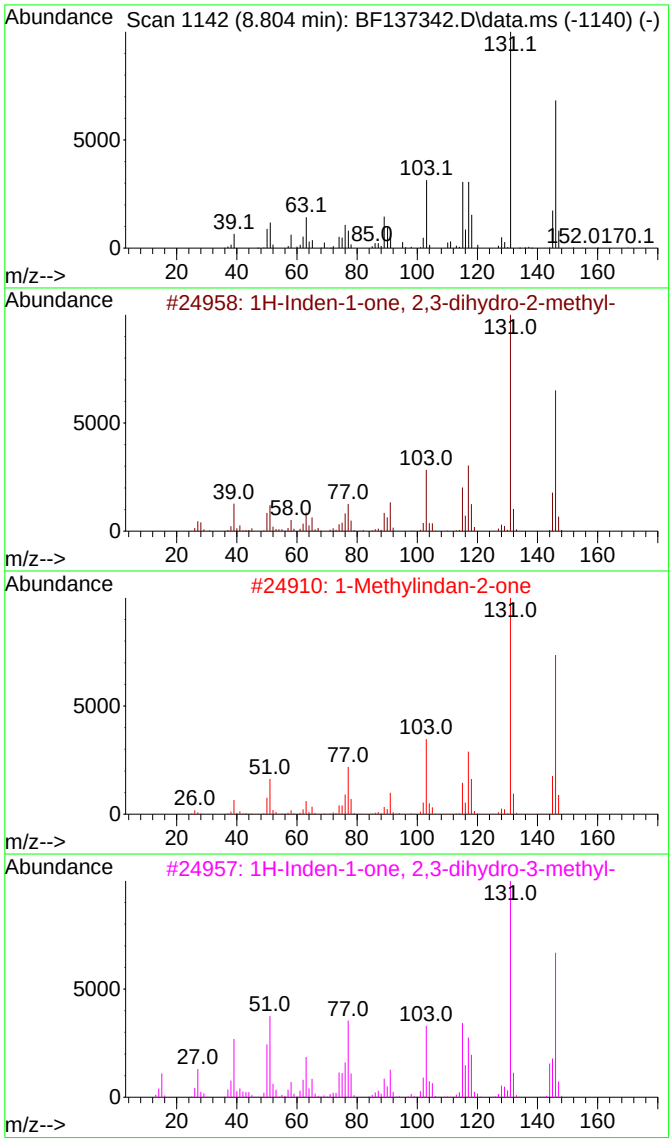
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

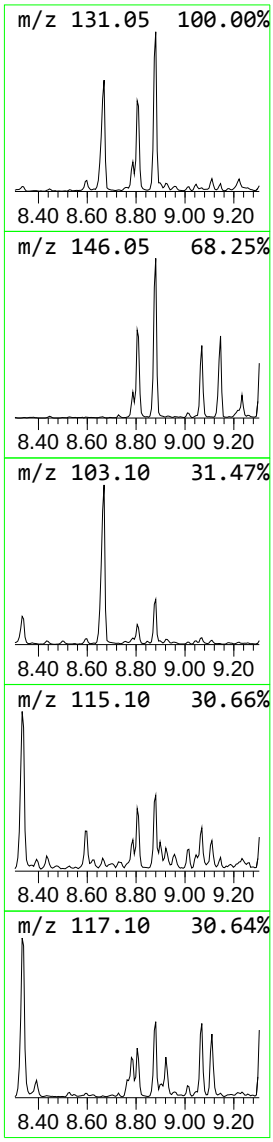
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 1H-Inden-1-one, 2,3-dihydro... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.804	17.72 ng	693730	Naphthalene-d8	8.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Inden-1-one, 2,3-dihydro-2-me...	146	C10H10O	017496-14-9	94
2	1-Methylindan-2-one	146	C10H10O	035587-60-1	91
3	1H-Inden-1-one, 2,3-dihydro-3-me...	146	C10H10O	006072-57-7	64
4	Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	58
5	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	58





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

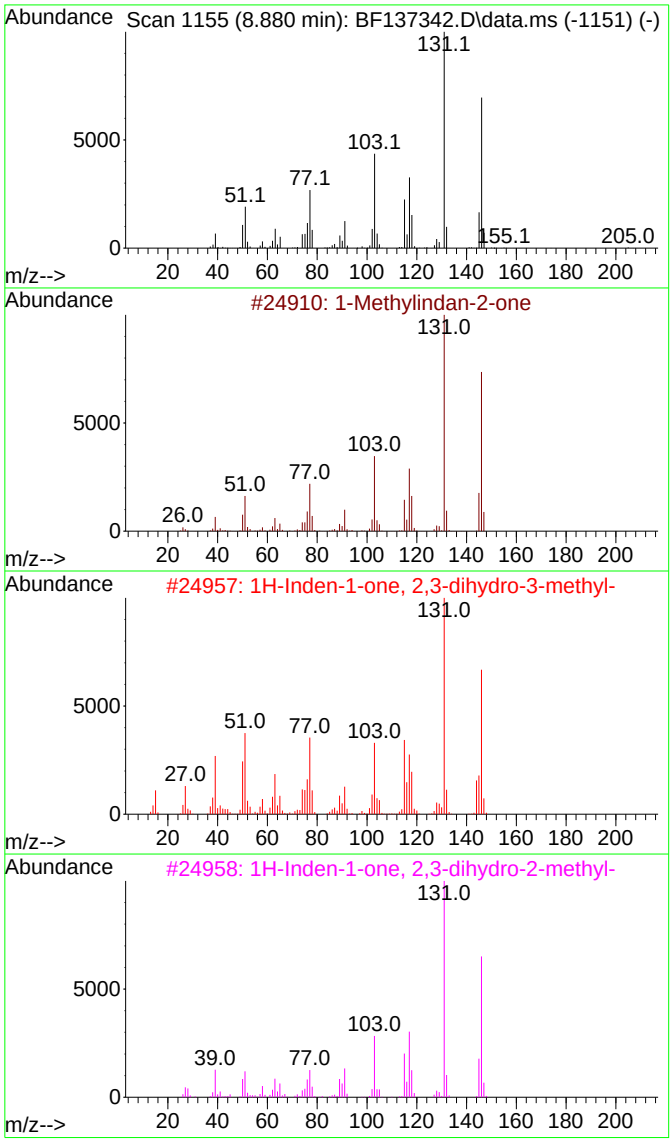
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

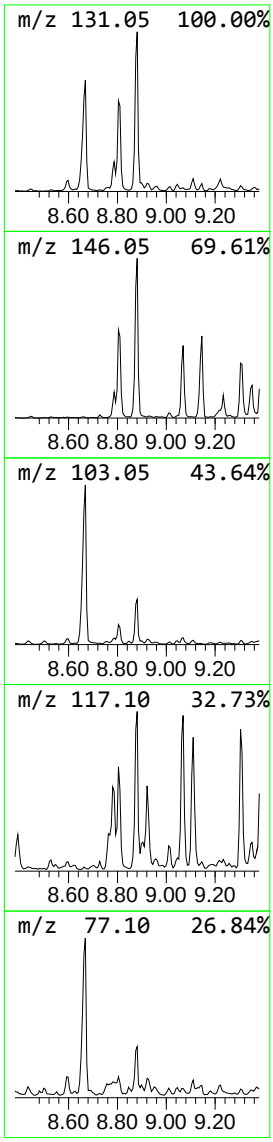
****

Peak Number 13 1-Methylindan-2-one Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.880	27.86 ng	1090450	Naphthalene-d8	8.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methylindan-2-one	146	C10H10O	035587-60-1	96
2	1H-Inden-1-one, 2,3-dihydro-3-me...	146	C10H10O	006072-57-7	91
3	1H-Inden-1-one, 2,3-dihydro-2-me...	146	C10H10O	017496-14-9	90
4	3-Buten-2-one, 4-phenyl-, (E)-	146	C10H10O	001896-62-4	76
5	1-Phenyldodec-1-en-3-one	258	C18H26O	872268-56-9	64





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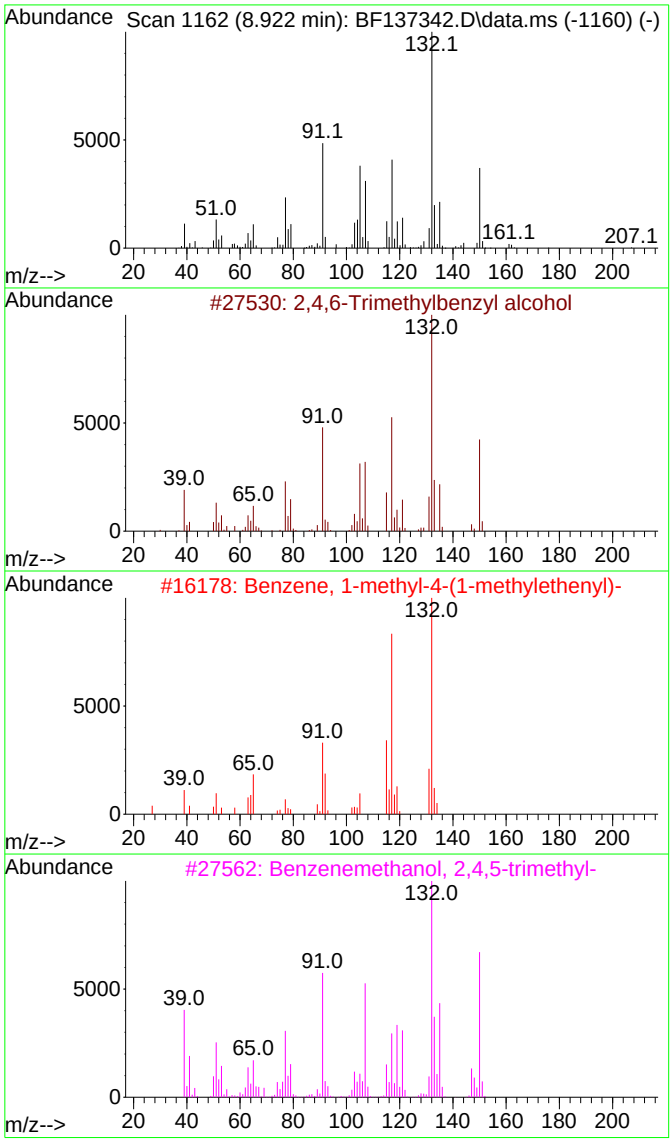
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

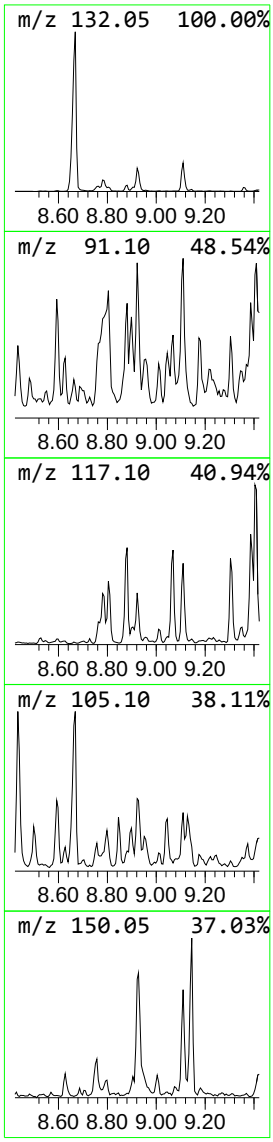
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 2,4,6-Trimethylbenzyl alcohol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.922	13.90 ng	543956	Naphthalene-d8	8.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,6-Trimethylbenzyl alcohol	150	C10H14O	1000342-65-8	59
2	Benzene, 1-methyl-4-(1-methyleth...	132	C10H12	001195-32-0	46
3	Benzenemethanol, 2,4,5-trimethyl-	150	C10H14O	004393-05-9	43
4	Benzene, 4-ethenyl-1,2-dimethyl-	132	C10H12	027831-13-6	43
5	1-Aminoindan	133	C9H11N	034698-41-4	43





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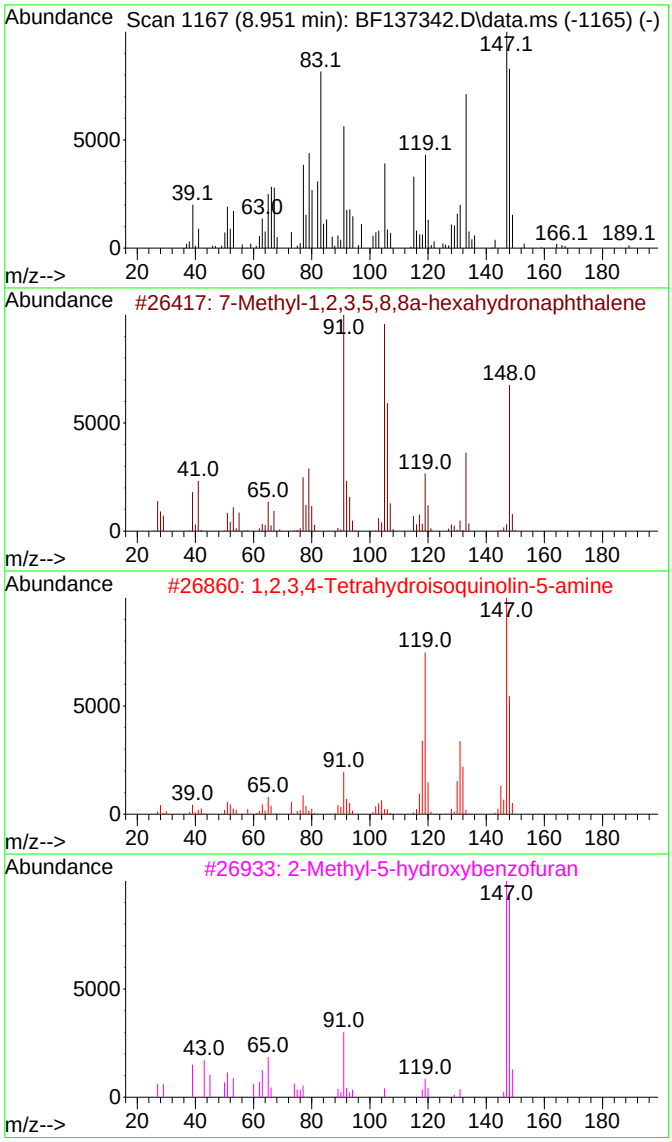
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

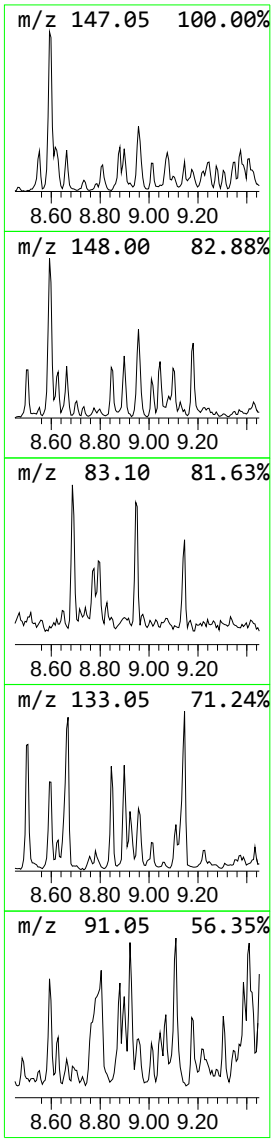
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 unknown8.951 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.951	9.93 ng	441969	Acenaphthene-d10	9.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Methyl-1,2,3,5,8,8a-hexahydron...	148	C11H16	107914-88-5	43
2	1,2,3,4-Tetrahydroisoquinolin-5-...	148	C9H12N2	115955-90-3	42
3	2-Methyl-5-hydroxybenzofuran	148	C9H8O2	006769-56-8	42
4	exo-7-(trans-1-Propenyl)bicyclo[...	148	C11H16	107983-42-6	41
5	Benzaldehyde, 2,4,5-trimethyl-	148	C10H12O	005779-72-6	38





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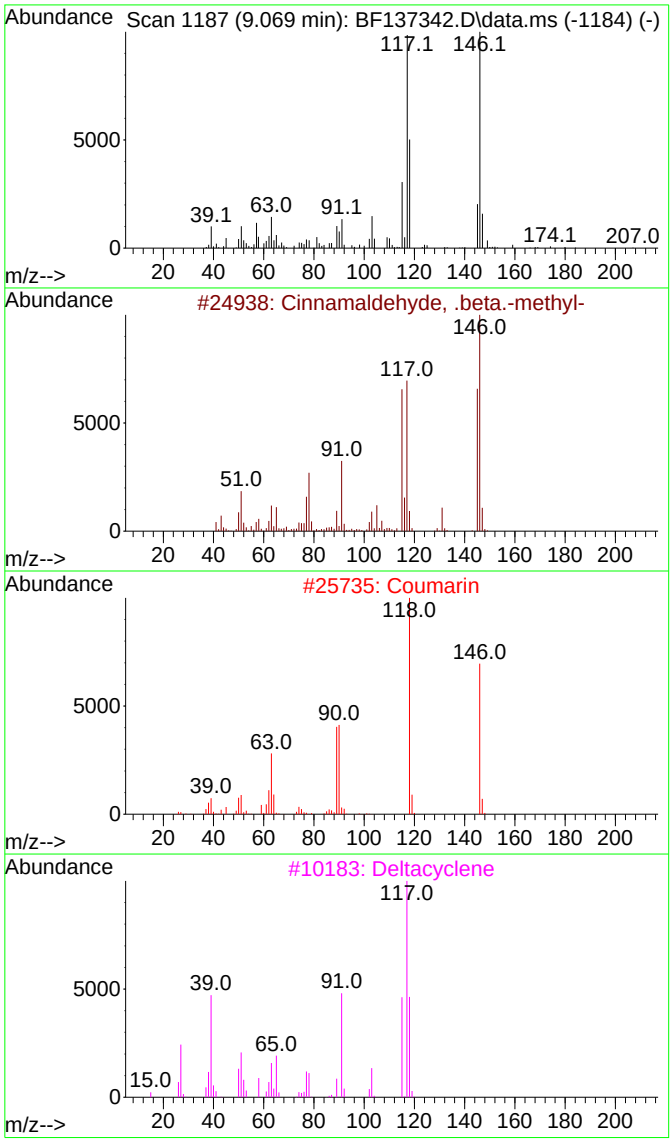
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

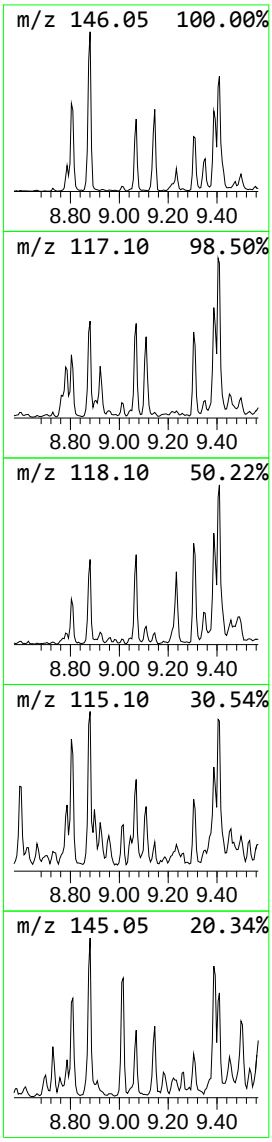
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 16 Cinnamaldehyde, .beta.-methyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.069	8.86 ng	394577	Acenaphthene-d10	9.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cinnamaldehyde, .beta.-methyl-	146	C10H10O	001196-67-4	58
2	Coumarin	146	C9H6O2	000091-64-5	45
3	Deltacyclene	118	C9H10	007785-10-6	43
4	2(1H)-Quinazolinone	146	C8H6N2O	007471-58-1	43
5	Indane	118	C9H10	000496-11-7	38





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Data File : BF137342.D
Acq On : 08 Feb 2024 17:21
Operator : CG\JU
Sample : P1342-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323P-GW-20240131-1

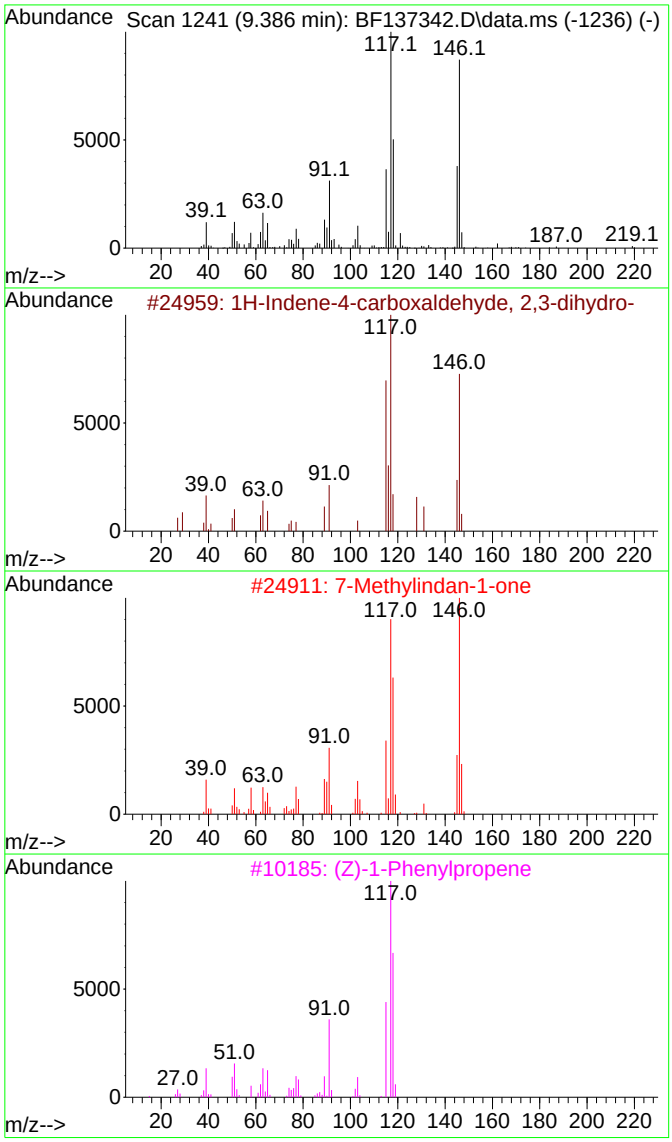
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

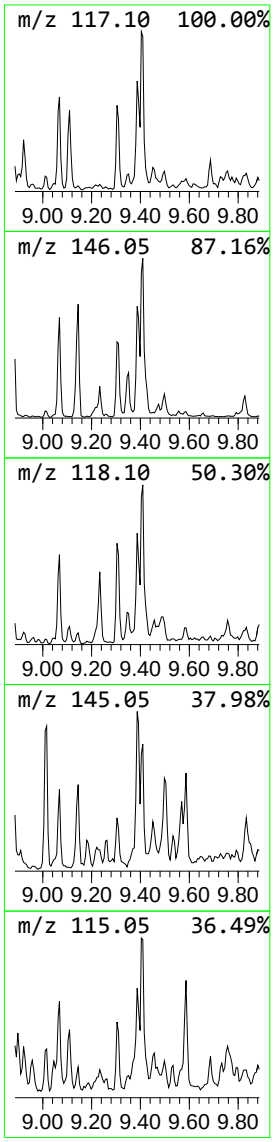
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 17 1H-Indene-4-carboxaldehyde,... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.386	11.10 ng	494305	Acenaphthene-d10	9.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene-4-carboxaldehyde, 2,3-...	146	C10H10O	051932-70-8	68
2	7-Methylindan-1-one	146	C10H10O	039627-61-7	68
3	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	64
4	Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
5	Indane	118	C9H10	000496-11-7	50





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Data File : BF137342.D
Acq On : 08 Feb 2024 17:21
Operator : CG\JU
Sample : P1342-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323P-GW-20240131-1

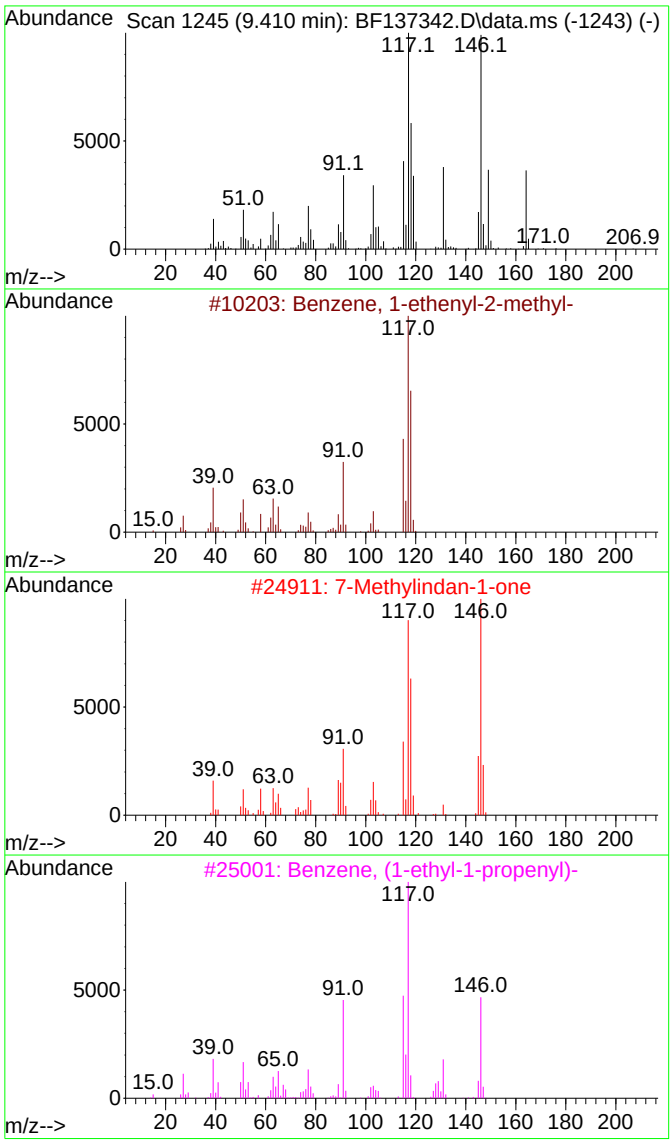
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

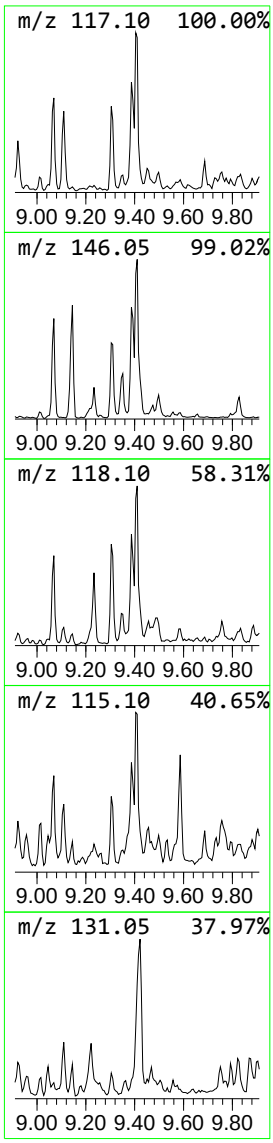
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 18 Benzene, 1-ethenyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.410	19.99 ng	889985	Acenaphthene-d10	9.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	76
2	7-Methylindan-1-one	146	C10H10O	039627-61-7	64
3	Benzene, (1-ethyl-1-propenyl)-	146	C11H14	004701-36-4	58
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	118	C9H10	022250-74-4	48
5	Benzoimidazole-1-carbaldehyde	146	C8H6N2O	1000294-58-3	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
Data File : BF137342.D
Acq On : 08 Feb 2024 17:21
Operator : CG\JU
Sample : P1342-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323P-GW-20240131-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

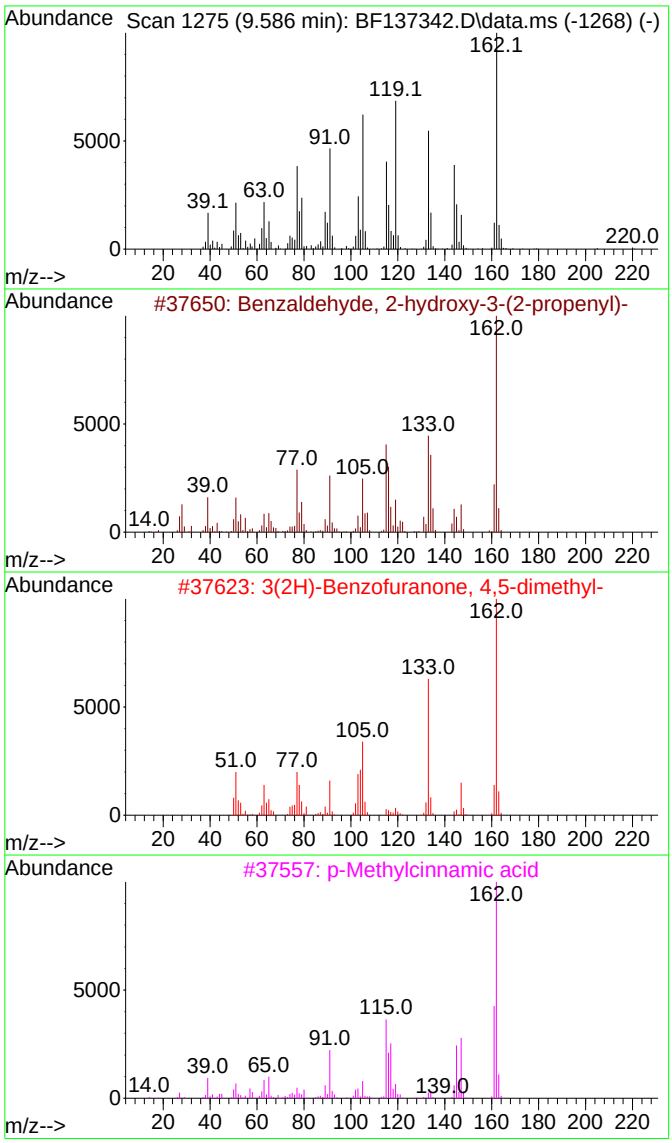
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

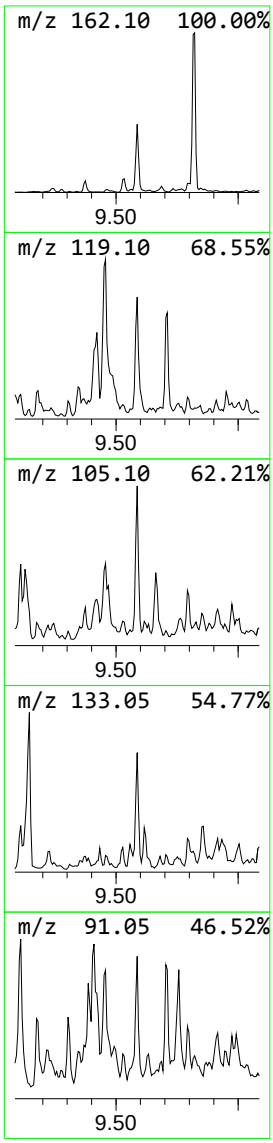
****

Peak Number 19 unknown9.586 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.586	16.85 ng	750219	Acenaphthene-d10	9.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 2-hydroxy-3-(2-pro...	162	C10H10O2	024019-66-7	49
2	3(2H)-Benzofuranone, 4,5-dimethyl-	162	C10H10O2	020895-42-5	38
3	p-Methylcinnamic acid	162	C10H10O2	001866-39-3	38
4	1,4-Benzenedicarboxaldehyde, 2,5...	162	C10H10O2	007044-92-0	38
5	Benzofuran-2-carboxylic acid	162	C9H6O3	000496-41-3	30





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Acq On : 08 Feb 2024 17:21
Operator : CG\JU
Sample : P1342-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323P-GW-20240131-1

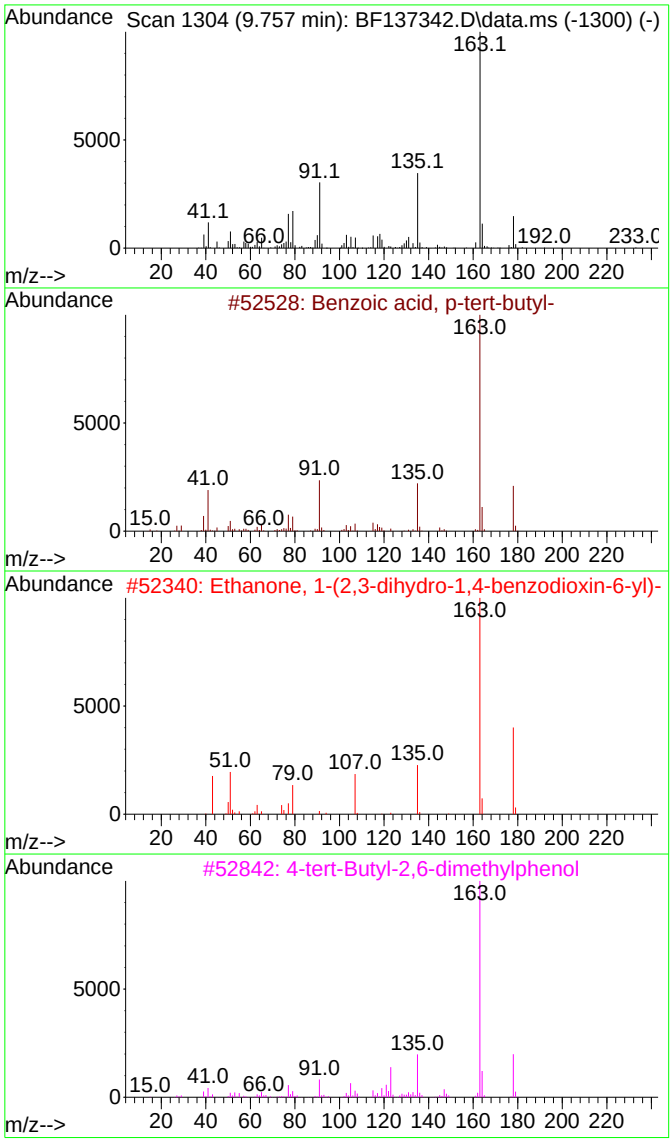
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

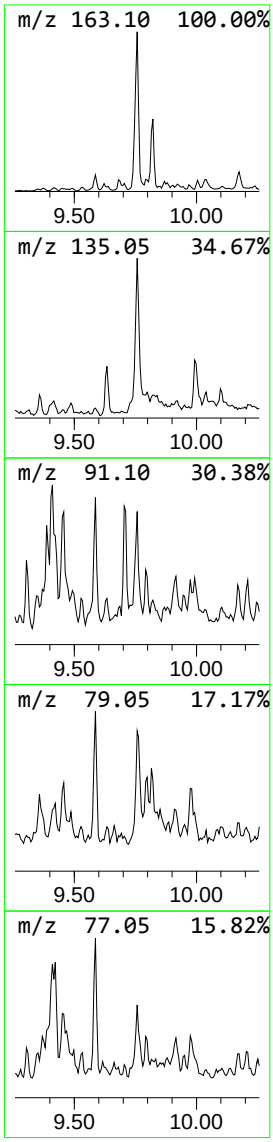
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 20 Benzoic acid, p-tert-butyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.757	10.22 ng	454997	Acenaphthene-d10	9.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	90
2	Ethanone, 1-(2,3-dihydro-1,4-ben...	178	C10H10O3	002879-20-1	74
3	4-tert-Butyl-2,6-dimethylphenol	178	C12H18O	000879-97-0	72
4	2-tert-Butyl-4-ethylphenol, O-is...	264	C16H24O3	1000487-42-5	72
5	Propofol	178	C12H18O	002078-54-8	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
Data File : BF137342.D
Acq On : 08 Feb 2024 17:21
Operator : CG\JU
Sample : P1342-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323P-GW-20240131-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Butanol, 2,3-...	3.116	18.9	ng	644856	1	6.781	681023	20.0
unknown7.110	7.110	8.4	ng	287221	1	6.781	681023	20.0
unknown7.634	7.634	14.3	ng	561122	2	8.063	782819	20.0
unknown8.186	8.186	8.9	ng	346726	2	8.063	782819	20.0
1H-Inden-1-ol, ...	8.333	69.2	ng	2709810	2	8.063	782819	20.0
2-Indanol	8.433	8.6	ng	335283	2	8.063	782819	20.0
Ethanone, 1-(4-...	8.498	8.4	ng	328389	2	8.063	782819	20.0
unknown8.592	8.592	13.8	ng	541033	2	8.063	782819	20.0
1H-Inden-1-one,...	8.669	90.4	ng	3538310	2	8.063	782819	20.0
unknown8.739	8.739	8.8	ng	343677	2	8.063	782819	20.0
unknown8.786	8.786	19.1	ng	747231	2	8.063	782819	20.0
1H-Inden-1-one,...	8.804	17.7	ng	693730	2	8.063	782819	20.0
1-Methylindan-2...	8.880	27.9	ng	1090450	2	8.063	782819	20.0
2,4,6-Trimethyl...	8.922	13.9	ng	543956	2	8.063	782819	20.0
unknown8.951	8.951	9.9	ng	441969	3	9.822	890416	20.0
Cinnamaldehyde,...	9.069	8.9	ng	394577	3	9.822	890416	20.0
1H-Indene-4-car...	9.386	11.1	ng	494305	3	9.822	890416	20.0
Benzene, 1-ethe...	9.410	20.0	ng	889985	3	9.822	890416	20.0
unknown9.586	9.586	16.9	ng	750219	3	9.822	890416	20.0
Benzoic acid, p...	9.757	10.2	ng	454997	3	9.822	890416	20.0