LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
Data File : BF137341.D
Acq On : 08 Feb 2024 16:52
Operator : CG\JU
Sample : P1342-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323P-GW-20240131-0

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: BF137341.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.122	169	176	181	rBV	331468	580507	16.24%	1.526%
2	3.657	258	267	274	rVB3	76691	143123	4.00%	0.376%
3	3.834	292	297	302	rBV	40110	57475	1.61%	0.151%
4	4.128	340	347	352	rBV	60348	82851	2.32%	0.218%
5	4.345	382	384	389	rVB3	59932	70492	1.97%	0.185%
6	4.557	412	420	428	rBV	52695	70890	1.98%	0.186%
7	4.922	476	482	487	rBV3	30376	73305	2.05%	0.193%
8	5.075	503	508	513	rVV5	60790	116582	3.26%	0.307%
9	5.134	513	518	526	rVB3	42300	59289	1.66%	0.156%
10	5.416	562	566	575	rBV	1396080	1303367	36.45%	3.427%
11	6.116	678	685	688	rBV3	70007	93868	2.63%	0.247%
12	6.216	698	702	709	rVB6	46011	71122	1.99%	0.187%
13	6.298	711	716	720	rBV2	52878	58288	1.63%	0.153%
14	6.381	727	730	733	rBV3	62844	66831	1.87%	0.176%
15	6.416	733	736	743	rVV	878884	838415	23.45%	2.205%
16	6.710	783	786	789	rBV2	66876	79307	2.22%	0.209%
17	6.781	795	798	802	rBV	761097	754759	21.11%	1.985%
18	6.816	802	804	806	rVV	212297	183003	5.12%	0.481%
19	6.839	806	808	813	rVB2	175874	174825	4.89%	0.460%
20	6.928	821	823	826	rBV	131561	122373	3.42%	0.322%
21	6.975	826	831	832	rVV3	101837	158057	4.42%	0.416%
22	7.033	836	841	844	rVV3	200764	360511	10.08%	0.948%
23	7.110	850	854	863	rBV4	169401	272740	7.63%	0.717%
24	7.186	863	867	871	rBV4	44175	80957	2.26%	0.213%
25	7.251	874	878	882	rVV2	96079	117207	3.28%	0.308%
26	7.345	886	894	898	rVV	2084247	2836117	79.32%	7.458%
27	7.381	898	900	904	rVV2	289559	381652	10.67%	1.004%
28	7.428	904	908	911	rVV4	79917	163267	4.57%	0.429%
29	7.463	911	914	917	rVV4	121556	144621	4.04%	0.380%
30	7.510	917	922	926	rVV3	149429	210586	5.89%	0.554%
31	7.551	926	929	932	rVB3	117238	104455	2.92%	0.275%
32	7.633	939	943	946	rVB2	318569	404906	11.32%	1.065%
33	7.675	948	950	953	rVB2	74572	63808	1.78%	0.168%
34	7.698	953	954	959	rVB5	61882	70061	1.96%	0.184%
35	7.751	960	963	967	rVB3	72051	82217	2.30%	0.216%
36	7.798	967	971	976	rBV4	144549	225916	6.32%	0.594%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
Data File : BF137341.D
Acq On : 08 Feb 2024 16:52
Operator : CG\JU
Sample : P1342-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323P-GW-20240131-0

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

37	7.898	985	988	991	rBV5	89173	106594	2.98%	0.280%
38	7.945	991	996	998	rBV5	121824	178158	4.98%	0.468%
39	7.998	1001	1005	1009	rVB3	153134	207993	5.82%	0.547%
40	8.063	1012	1016	1018	rBV	1059040	934737	26.14%	2.458%
41	8.110	1022	1024	1030	rVB5	88847	114655	3.21%	0.301%
42	8.186	1032	1037	1040	rBV2	221673	291159	8.14%	0.766%
43	8.239	1040	1046	1049	rVB6	110186	192950	5.40%	0.507%
44	8.292	1049	1055	1058	rBV4	250032	438835	12.27%	1.154%
45	8.333	1058	1062	1066	rVV	1647633	1549949	43.35%	4.076%
46	8.433	1077	1079	1082	rBV	100480	107783	3.01%	0.283%
47	8.463	1082	1084	1087	rVV	113416	98428	2.75%	0.259%
48	8.498	1087	1090	1096	rVB3	152652	205615	5.75%	0.541%
49	8.551	1096	1099	1103	rVB5	104497	115341	3.23%	0.303%
50	8.592	1103	1106	1109	rBV2	329567	363950	10.18%	0.957%
51	8.663	1113	1118	1120	rVB	2063564	1876211	52.48%	4.934%
52	8.686	1120	1122	1124	rVB3	88936	57747	1.62%	0.152%
53	8.733	1127	1130	1132	rBV	161806	165420	4.63%	0.435%
54	8.804	1140	1142	1145	rVB	481250	364408	10.19%	0.958%
55	8.845	1147	1149	1151	rBV	129648	85420	2.39%	0.225%
56	8.875	1151	1154	1156	rBV	722561	565866	15.83%	1.488%
57	8.898	1156	1158	1160	rVV2	198735	173358	4.85%	0.456%
58	8.922	1160	1162	1165	rVV2	359810	329338	9.21%	0.866%
59	8.951	1165	1167	1173	rVB4	244602	344000	9.62%	0.905%
60	9.010	1173	1177	1180	rBV2	212579	243540	6.81%	0.640%
61	9.045	1180	1183	1184	rBV	161782	154529	4.32%	0.406%
62	9.063	1184	1186	1190	rVB3	317890	280541	7.85%	0.738%
63	9.110	1190	1194	1196	rBV	329241	310737	8.69%	0.817%
64	9.145	1196	1200	1203	rVB	4071261	3575385	100.00%	9.402%
65	9.175	1203	1205	1209	rBV3	88860	103280	2.89%	0.272%
66	9.216	1209	1212	1214	rBV2	102944	101811	2.85%	0.268%
67	9.263	1218	1220	1224	rVB4	94810	115731	3.24%	0.304%
68	9.304	1224	1227	1230	rBV2	302863	262405	7.34%	0.690%
69	9.345	1230	1234	1236	rBV2	174758	200202	5.60%	0.526%
70	9.386	1236	1241	1242	rBV2	271573	227002	6.35%	0.597%
71	9.404	1242	1244	1248	rVB3	496122	545430	15.26%	1.434%
72	9.451	1248	1252	1256	rBV	229721	278709	7.80%	0.733%
73	9.527	1263	1265	1268	rVB2	155934	125538	3.51%	0.330%
74	9.586	1268	1275	1279	rBV2	533789	611060	17.09%	1.607%
75	9.633	1281	1283	1287	rVB3	91886	81792	2.29%	0.215%
76	9.704	1293	1295	1297	rVB	161557	105674	2.96%	0.278%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
Data File : BF137341.D
Acq On : 08 Feb 2024 16:52
Operator : CG\JU
Sample : P1342-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323P-GW-20240131-0

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

77	9.757	1297	1304	1308	rBV2	409451	542715	15.18%	1.427%
78	9.792	1308	1310	1312	rVV2	221631	201220	5.63%	0.529%
79	9.816	1312	1314	1321	rVB	1104121	1043810	29.19%	2.745%
80	9.910	1327	1330	1334	rVB4	141483	170382	4.77%	0.448%
81	9.945	1334	1336	1338	rVV3	86836	68654	1.92%	0.181%
82	9.974	1338	1341	1347	rVB	212031	278645	7.79%	0.733%
83	10.169	1371	1374	1377	rVV4	184258	181122	5.07%	0.476%
84	10.204	1377	1380	1385	rVV4	122277	150200	4.20%	0.395%
85	10.251	1385	1388	1391	rVV3	100691	124868	3.49%	0.328%
86	10.286	1391	1394	1396	rVV2	80355	78985	2.21%	0.208%
87	10.433	1416	1419	1427	rVB2	269873	284974	7.97%	0.749%
88	10.610	1445	1449	1455	rBV	2147675	2132800	59.65%	5.608%
89	10.739	1468	1471	1479	rVB6	68197	111780	3.13%	0.294%
90	11.186	1544	1547	1549	rBV	90217	68718	1.92%	0.181%
91	11.310	1564	1568	1572	rVB	1032569	846180	23.67%	2.225%
92	11.604	1616	1618	1621	rBV	68103	57402	1.61%	0.151%
93	11.851	1657	1660	1669	rVB2	243218	253021	7.08%	0.665%
94	11.974	1678	1681	1684	rVB	81903	68842	1.93%	0.181%
95	12.645	1792	1795	1798	rBV2	78614	69636	1.95%	0.183%
96	12.910	1836	1840	1843	rBV	3176131	2849834	79.71%	7.494%
97	13.827	1993	1996	2006	rVB	70703	87081	2.44%	0.229%
98	13.962	2015	2019	2026	rBV	763244	678823	18.99%	1.785%
99	15.445	2266	2271	2277	rBV	609445	747067	20.89%	1.964%
100	17.162	2558	2563	2571	rVB	30649	64008	1.79%	0.168%

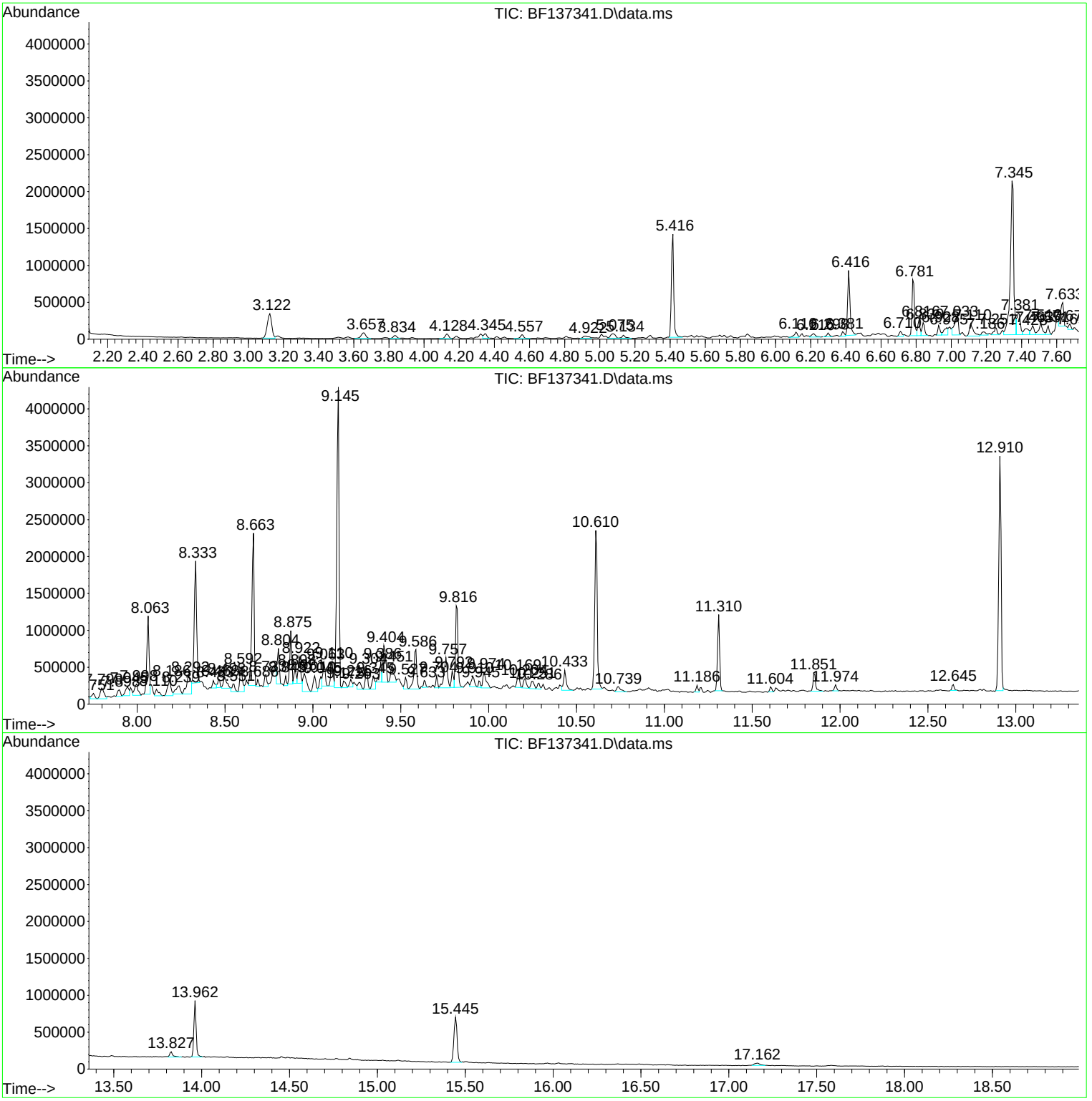
Sum of corrected areas: 38029798

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
Data File : BF137341.D
Acq On : 08 Feb 2024 16:52
Operator : CG\JU
Sample : P1342-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323P-GW-20240131-0

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\
Data File : BF137341.D
Acq On : 08 Feb 2024 16:52
Operator : CG\JU
Sample : P1342-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323P-GW-20240131-0

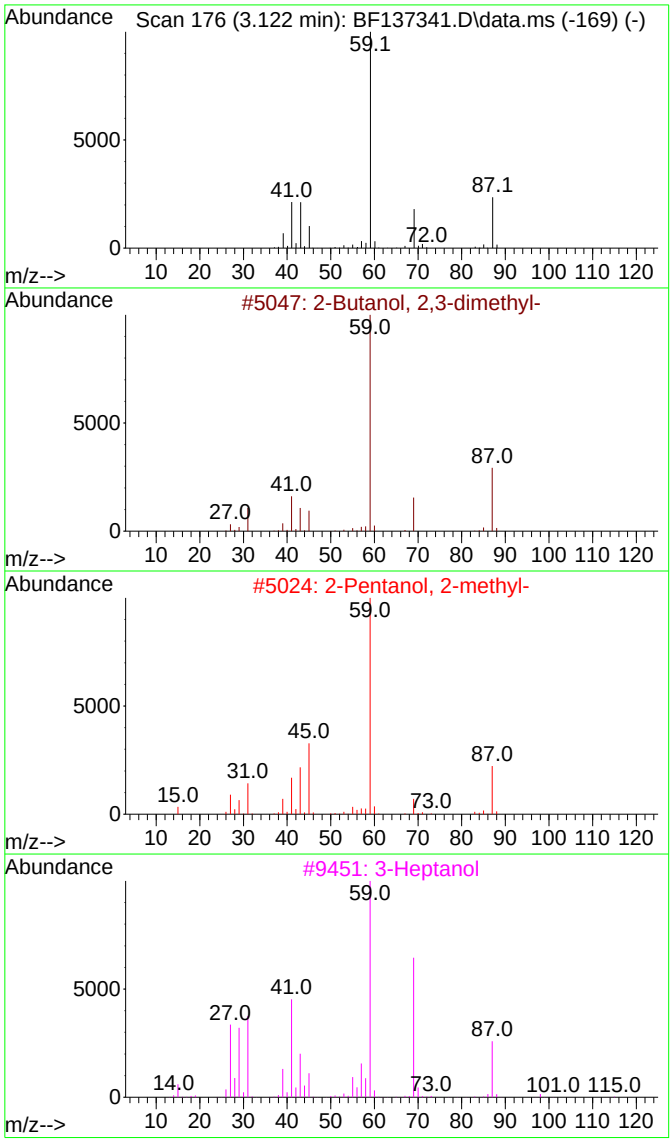
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

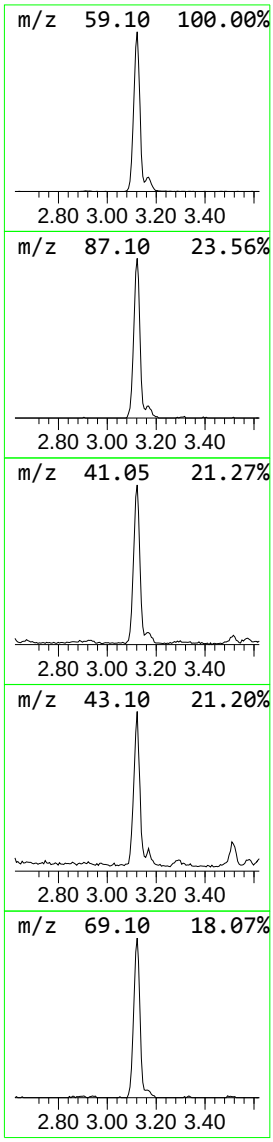
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.122	15.38 ng	580507	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	50
3	3-Heptanol	116	C7H16O	000589-82-2	40
4	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	38
5	2-Decanol, methyl ether	172	C11H24O	1000333-83-9	36





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
Data File : BF137341.D
Acq On : 08 Feb 2024 16:52
Operator : CG\JU
Sample : P1342-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323P-GW-20240131-0

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

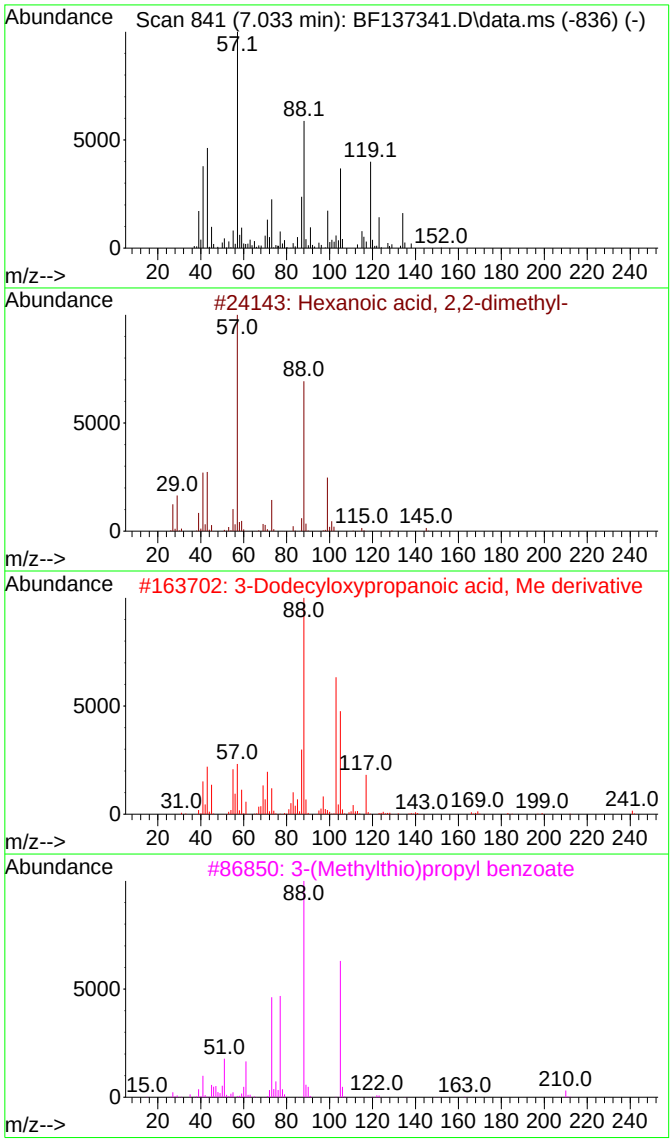
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

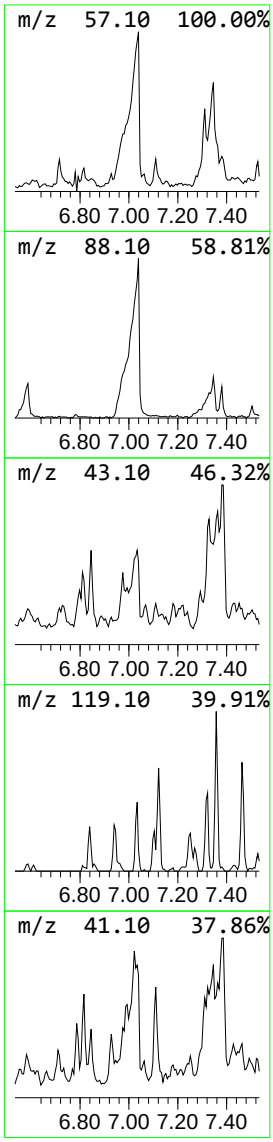
****

Peak Number 2 unknown7.033 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.033	9.55 ng	360511	1,4-Dichlorobenzene-d4	6.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2,2-dimethyl-	144	C8H16O2	000813-72-9	27
2	3-Dodecyloxypropanoic acid, Me d...	272	C16H32O3	1000497-89-8	25
3	3-(Methylthio)propyl benzoate	210	C11H14O2S	1000367-09-7	16
4	Methyl propionate	88	C4H8O2	000554-12-1	14
5	Hydrazine, 1,2-diethyl-	88	C4H12N2	001615-80-1	14





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
Data File : BF137341.D
Acq On : 08 Feb 2024 16:52
Operator : CG\JU
Sample : P1342-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323P-GW-20240131-0

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

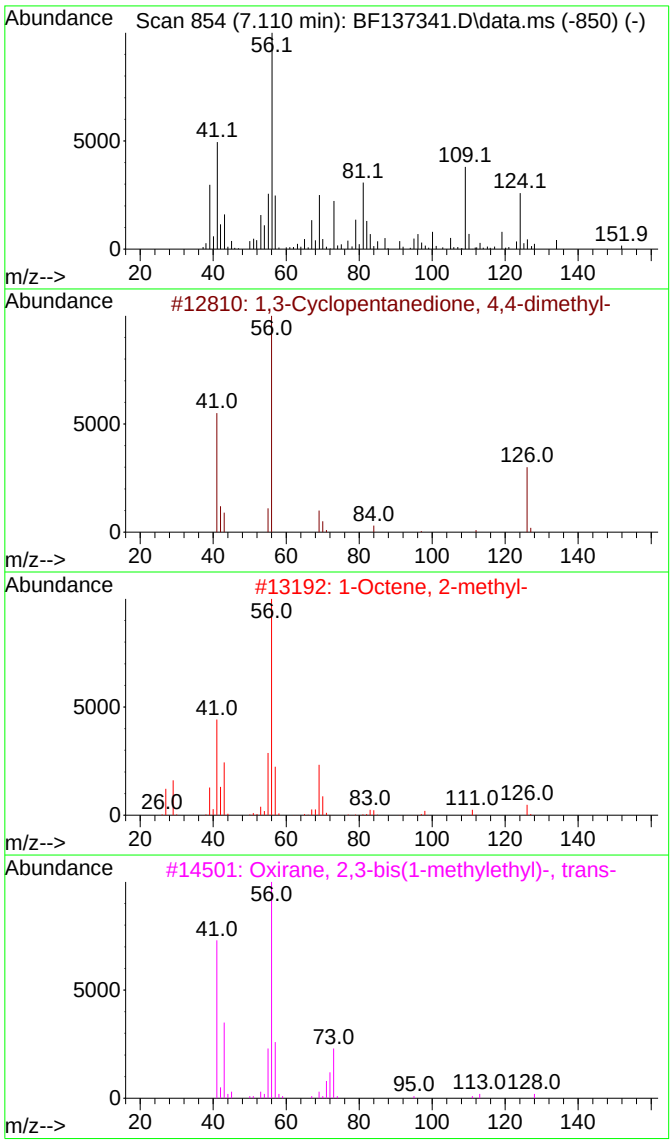
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

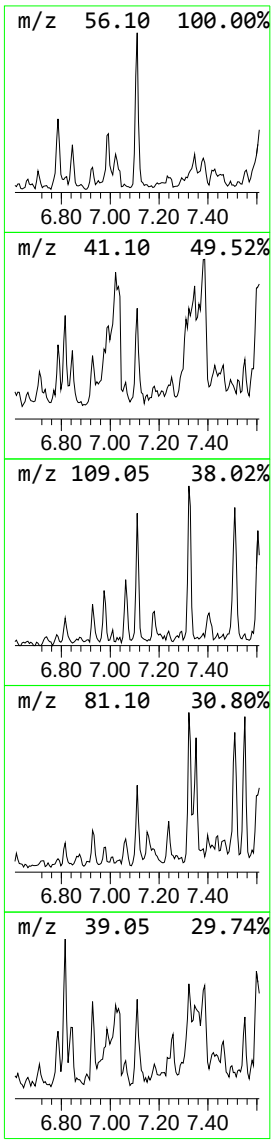
****

Peak Number 3 unknown7.110 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.110	7.23 ng	272740	1,4-Dichlorobenzene-d4	6.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 4,4-dimet...	126	C7H10O2	004683-51-6	43
2	1-Octene, 2-methyl-	126	C9H18	004588-18-5	43
3	Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	43
4	1-Octene, 7-methyl-	126	C9H18	013151-06-9	38
5	1-Heptene, 2,6-dimethyl-	126	C9H18	003074-78-0	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
Data File : BF137341.D
Acq On : 08 Feb 2024 16:52
Operator : CG\JU
Sample : P1342-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323P-GW-20240131-0

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

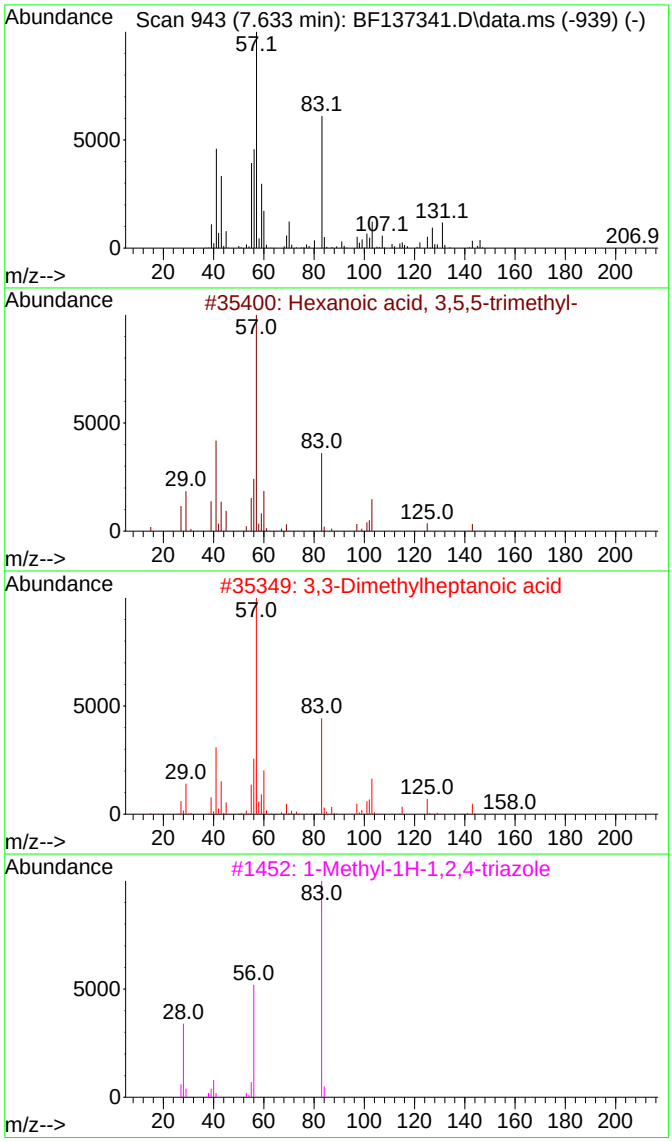
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

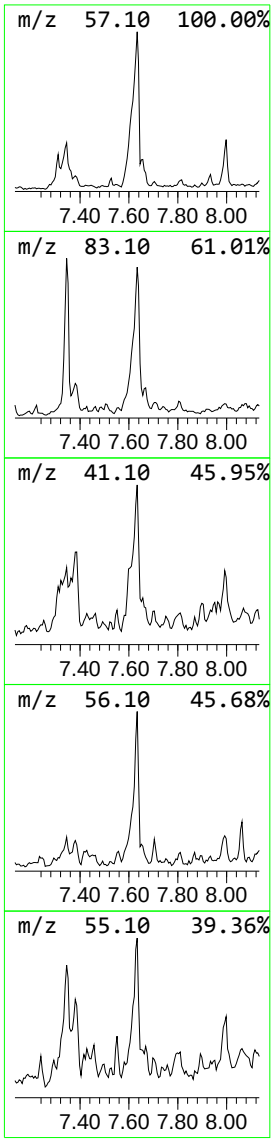
****

Peak Number 4 unknown7.633 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.633	8.66 ng	404906	Naphthalene-d8	8.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	38
2	3,3-Dimethylheptanoic acid	158	C9H18O2	067061-30-7	35
3	1-Methyl-1H-1,2,4-triazole	83	C3H5N3	006086-21-1	25
4	Hexanoyl chloride, 3,5,5-trimethyl-	176	C9H17ClO	036727-29-4	25
5	Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
Data File : BF137341.D
Acq On : 08 Feb 2024 16:52
Operator : CG\JU
Sample : P1342-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323P-GW-20240131-0

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

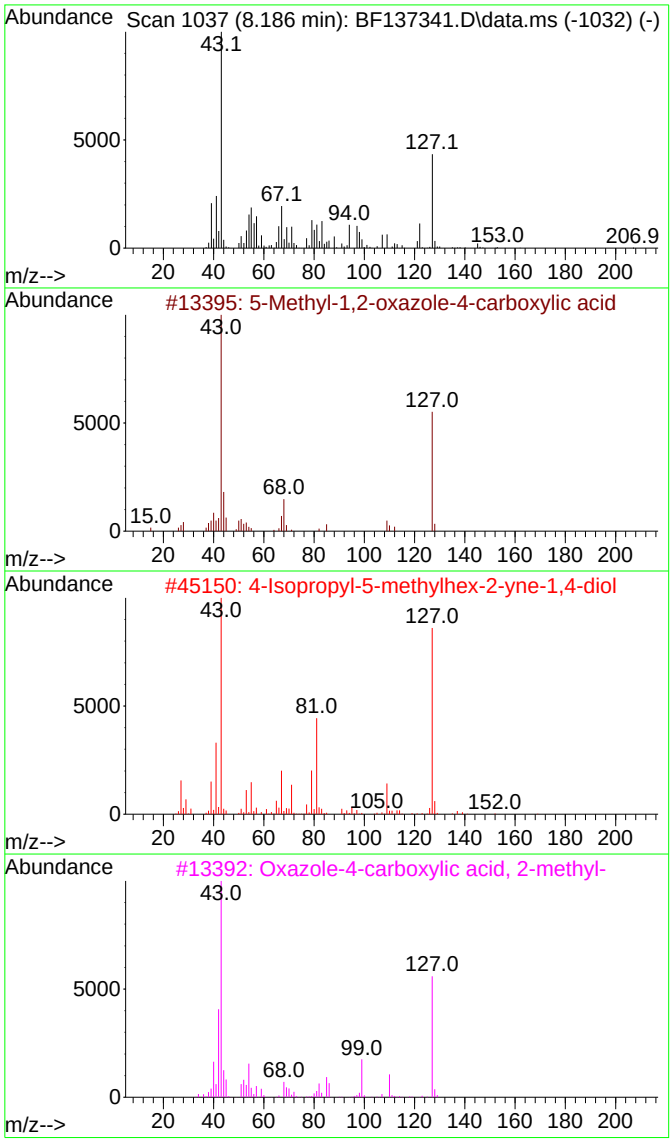
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

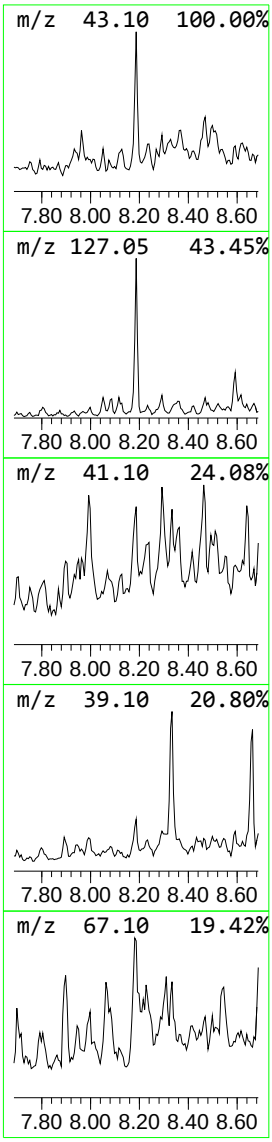
****

Peak Number 5 unknown8.186 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.186	6.23 ng	291159	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	4-Isopropyl-5-methylhex-2-yne-1,...	170	C10H18O2	070372-89-3	25
3	Oxazole-4-carboxylic acid, 2-met...	127	C5H5NO3	023012-17-1	22
4	4-Pentenoic acid, 2-acetyl-, eth...	170	C9H14O3	000610-89-9	17
5	Cyclohexanepropanol, 2-acetoxy-	200	C11H20O3	1000197-25-8	16





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
Data File : BF137341.D
Acq On : 08 Feb 2024 16:52
Operator : CG\JU
Sample : P1342-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323P-GW-20240131-0

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

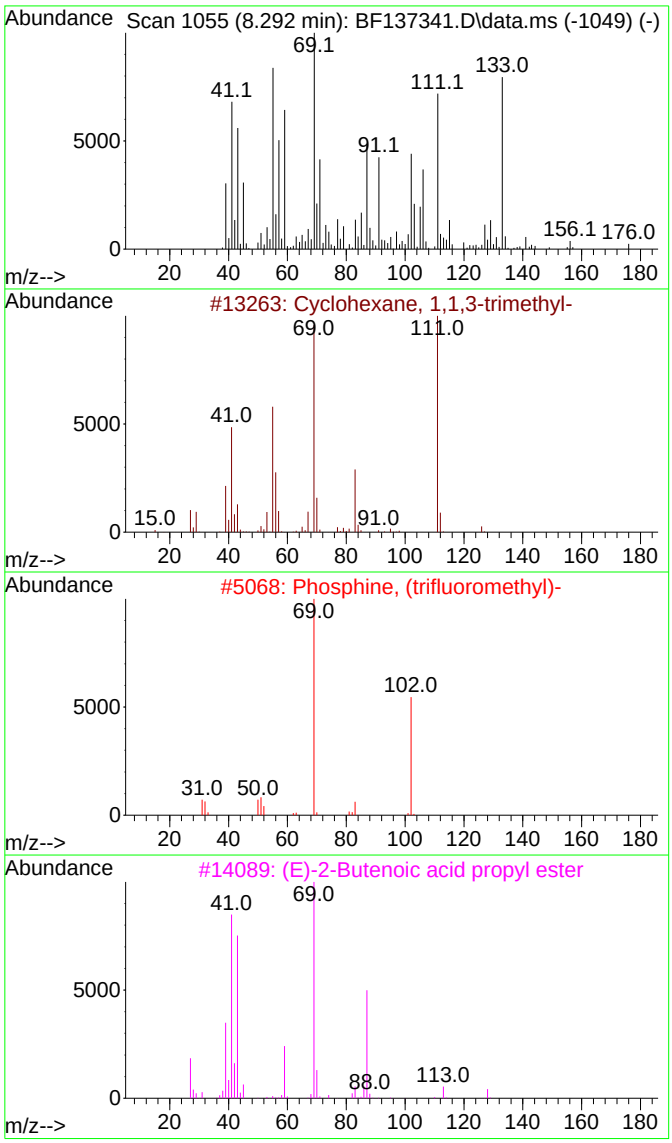
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

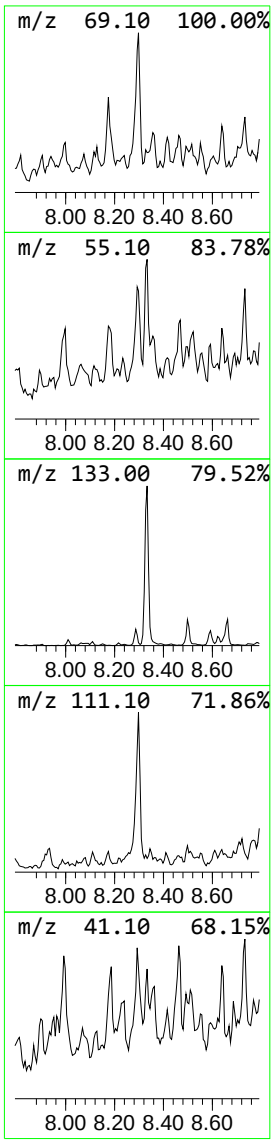
****

Peak Number 6 unknown8.292 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.292	9.39 ng	438835	Naphthalene-d8	8.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	20
2	Phosphine, (trifluoromethyl)-	102	CH2F3P	000420-52-0	18
3	(E)-2-Butenoic acid propyl ester	128	C7H12O2	010352-87-1	18
4	Cyclooctane, ethyl-	140	C10H20	013152-02-8	14
5	Cyclohexane, 1-ethyl-1,4-dimethy...	140	C10H20	062238-32-8	14





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
Data File : BF137341.D
Acq On : 08 Feb 2024 16:52
Operator : CG\JU
Sample : P1342-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323P-GW-20240131-0

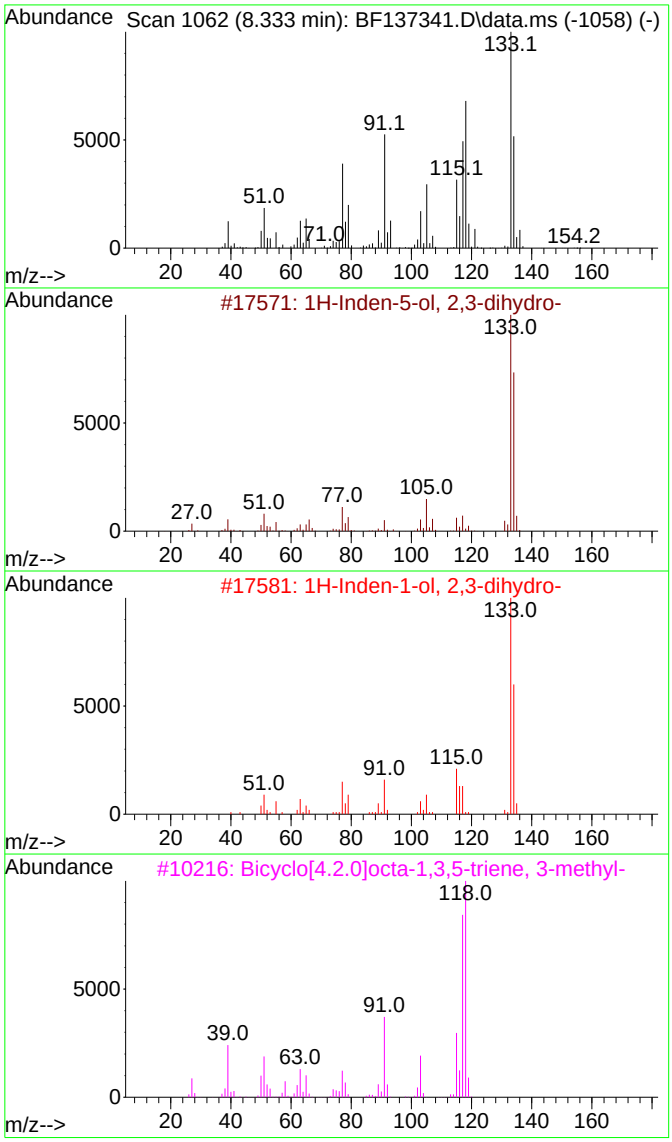
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

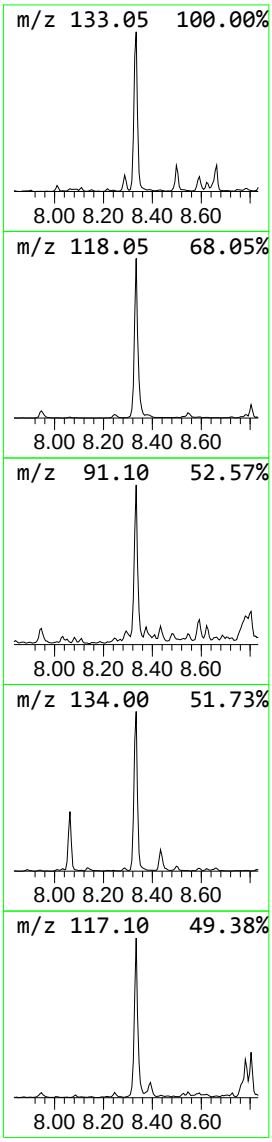
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1H-Inden-5-ol, 2,3-dihydro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.333	33.16 ng	1549950	Naphthalene-d8	8.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Inden-5-ol, 2,3-dihydro-	134	C9H10O	001470-94-6	50
2	1H-Inden-1-ol, 2,3-dihydro-	134	C9H10O	006351-10-6	46
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	118	C9H10	022250-74-4	41
4	Tetrahydroquinoxaline	134	C8H10N2	003476-89-9	38
5	1,4-Benzenedicarboxaldehyde	134	C8H6O2	000623-27-8	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
Data File : BF137341.D
Acq On : 08 Feb 2024 16:52
Operator : CG\JU
Sample : P1342-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323P-GW-20240131-0

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

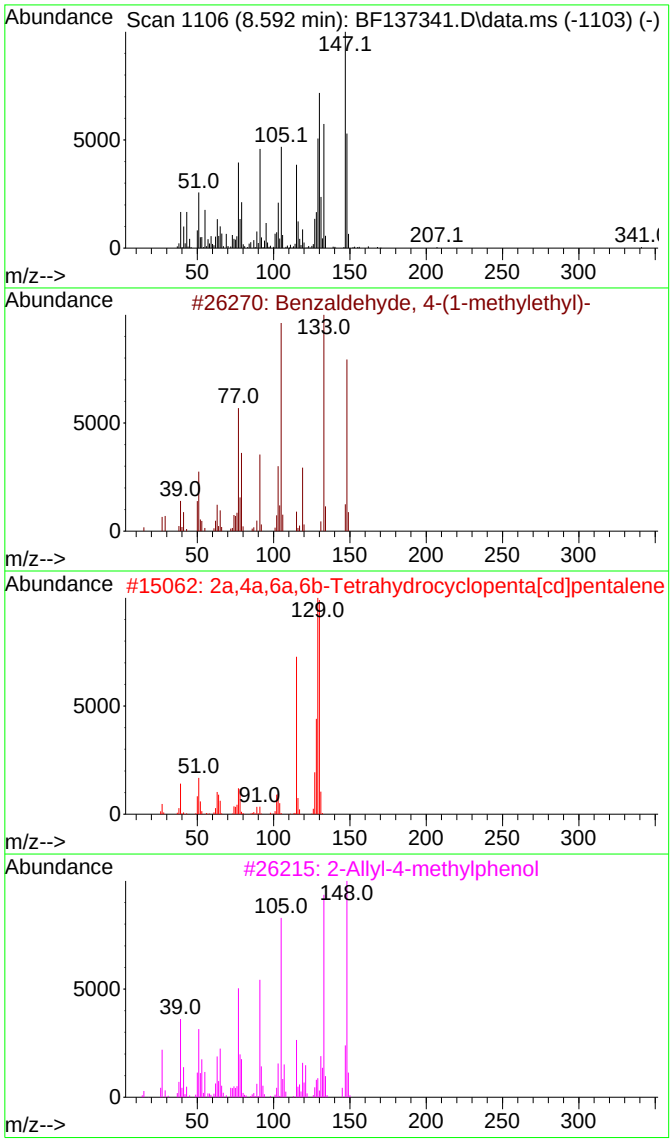
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

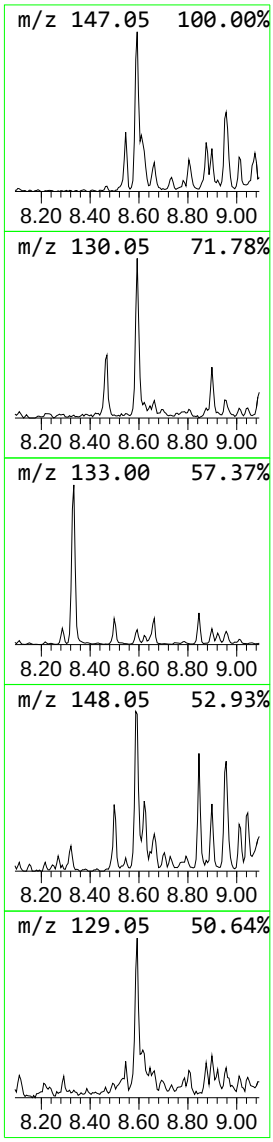
****

Peak Number 8 unknown8.592 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.592	7.79 ng	363950	Naphthalene-d8	8.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 4-(1-methylethyl)-	148	C10H12O	000122-03-2	38
2	2a,4a,6a,6b-Tetrahydrocyclopenta...	130	C10H10	006053-74-3	38
3	2-Allyl-4-methylphenol	148	C10H12O	006628-06-4	30
4	Benzene, 1,3-butadienyl-	130	C10H10	001515-78-2	30
5	Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
Data File : BF137341.D
Acq On : 08 Feb 2024 16:52
Operator : CG\JU
Sample : P1342-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323P-GW-20240131-0

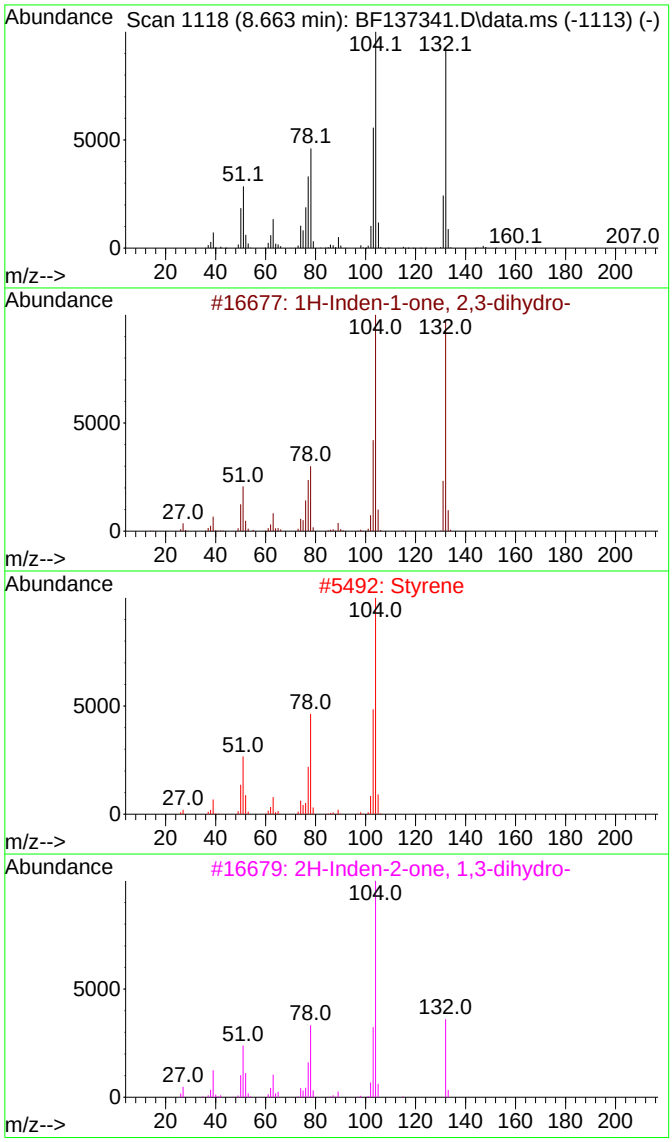
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

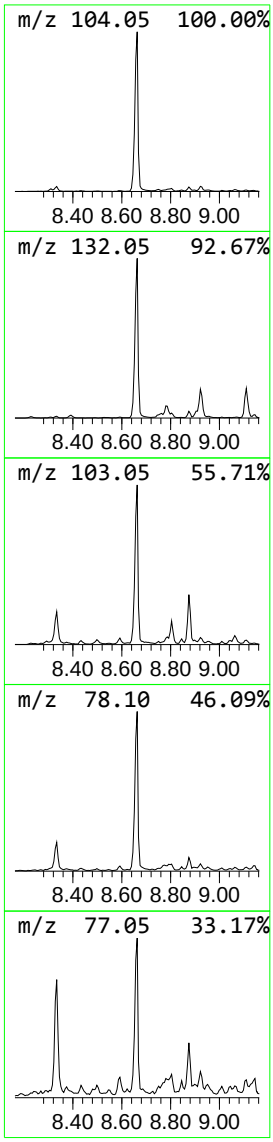
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.663	40.14 ng	1876210	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	94
2	Styrene	104	C8H8	000100-42-5	91
3	2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	68
4	Bicyclo[4.2.0]octa-1,3,5-triene	104	C8H8	000694-87-1	64
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	52





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
Data File : BF137341.D
Acq On : 08 Feb 2024 16:52
Operator : CG\JU
Sample : P1342-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323P-GW-20240131-0

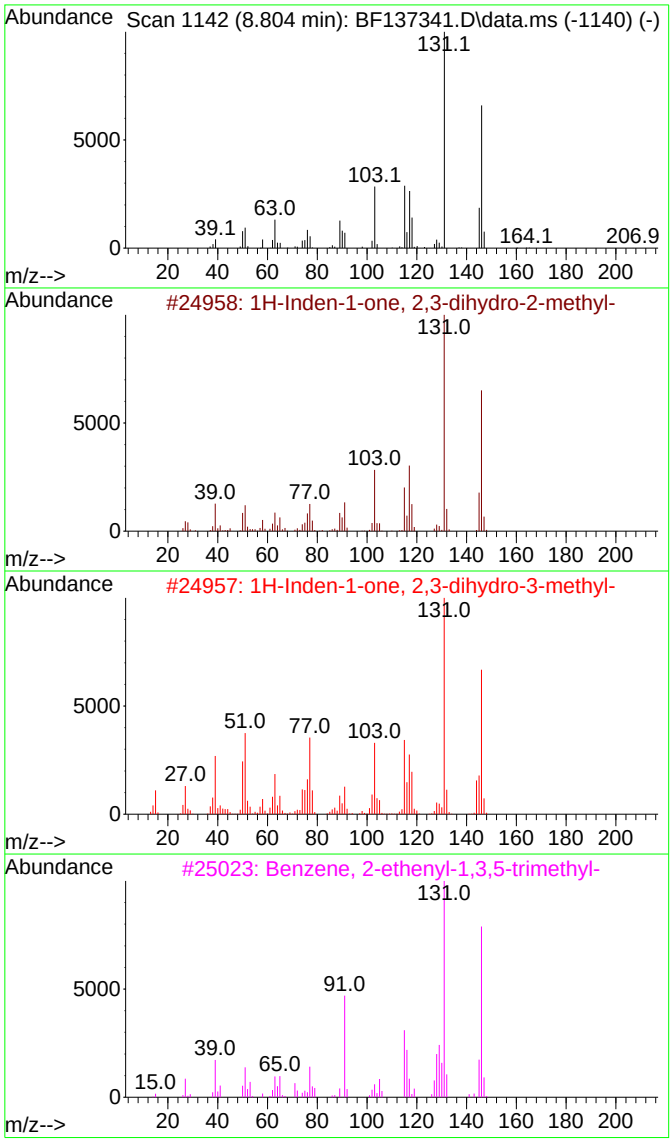
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

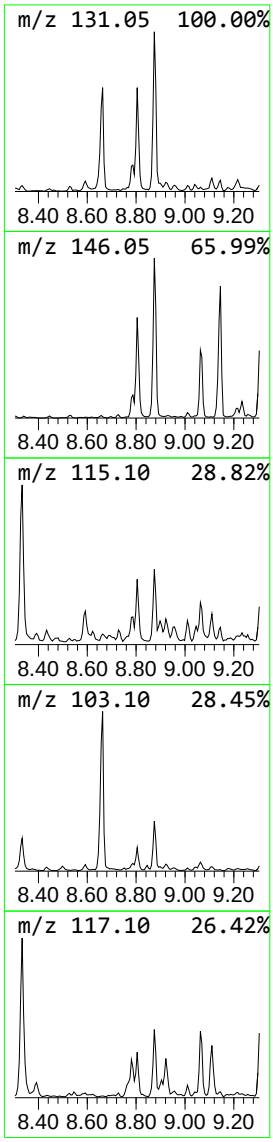
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1H-Inden-1-one, 2,3-dihydro... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.804	7.80 ng	364408	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	93
2	1H-Inden-1-one, 2,3-dihydro-3-me...	146	C10H10O	006072-57-7	90
3	Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	64
4	1-Methylindan-2-one	146	C10H10O	035587-60-1	62
5	Ethyl-2-benzofuran	146	C10H10O	003131-63-3	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
Data File : BF137341.D
Acq On : 08 Feb 2024 16:52
Operator : CG\JU
Sample : P1342-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323P-GW-20240131-0

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

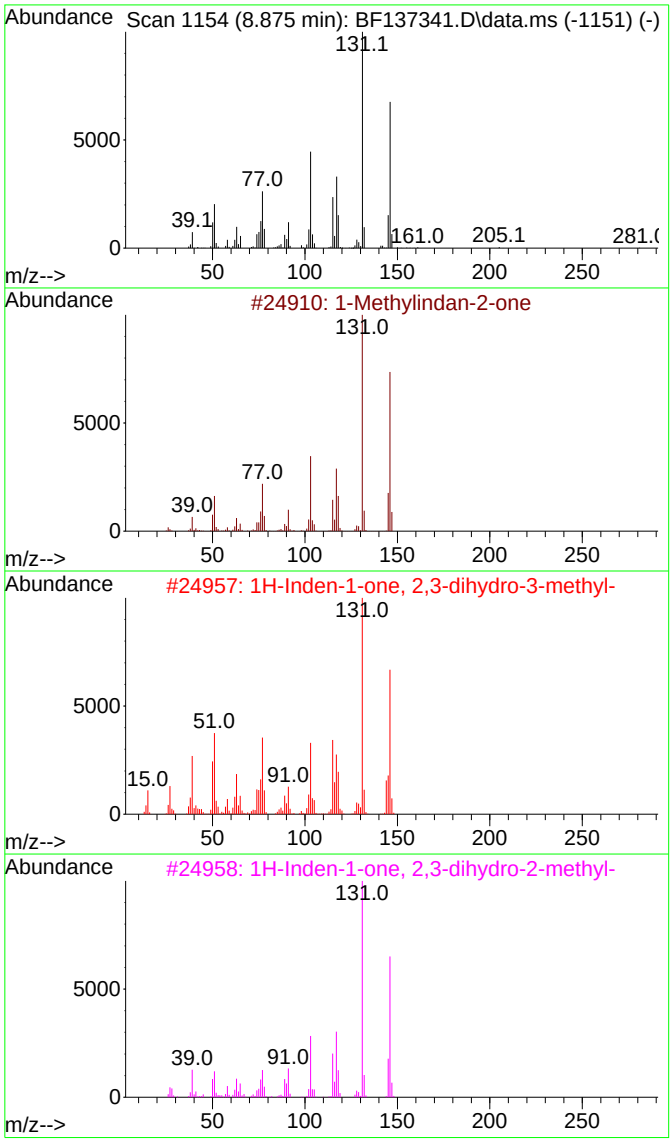
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

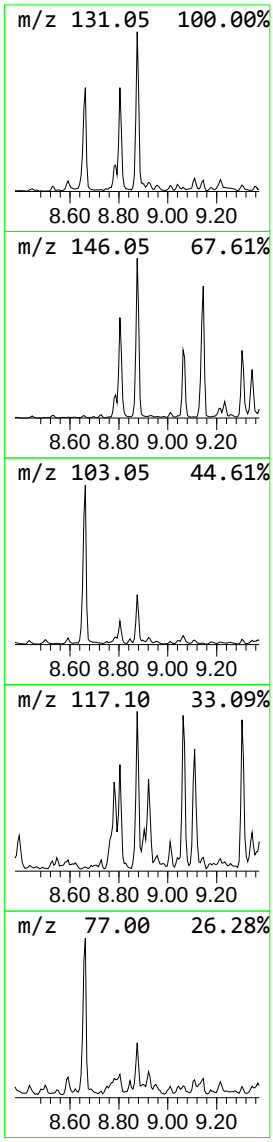
****

Peak Number 11 1-Methylindan-2-one Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.875	12.11 ng	565866	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	93
3	1H-Inden-1-one, 2,3-dihydro-2-me...	146	C10H10O	017496-14-9	74
4	1-Decen-3-one, 5-hydroxy-4-penty...	316	C21H32O2	959035-43-9	59
5	1-Phenyldodec-1-en-3-one	258	C18H26O	872268-56-9	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
Data File : BF137341.D
Acq On : 08 Feb 2024 16:52
Operator : CG\JU
Sample : P1342-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323P-GW-20240131-0

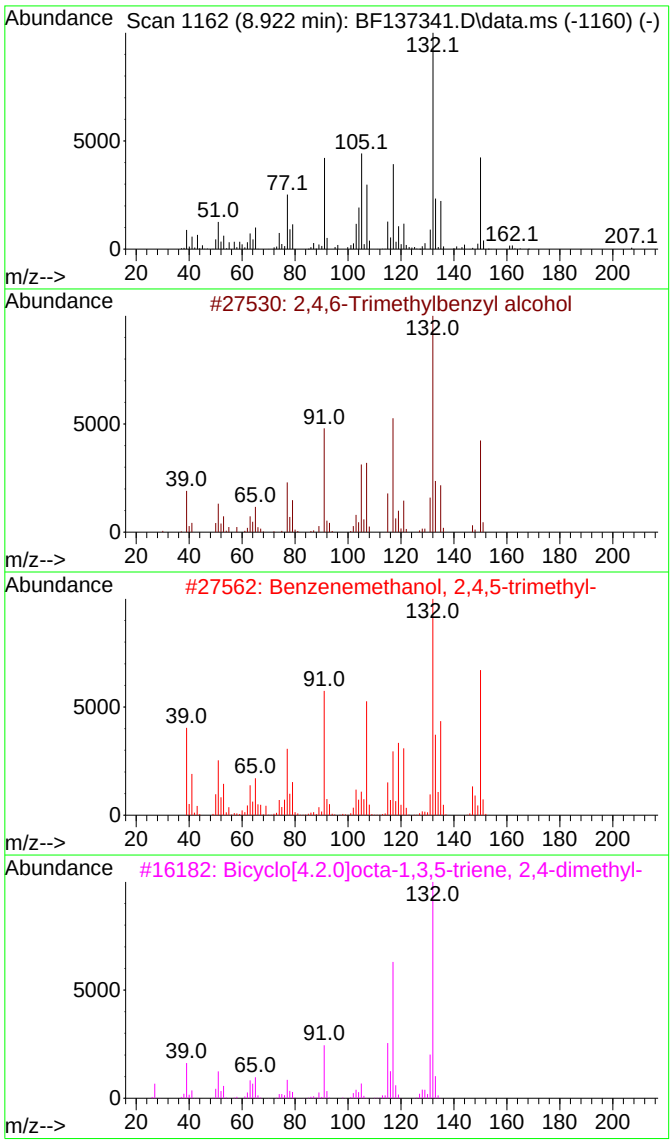
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

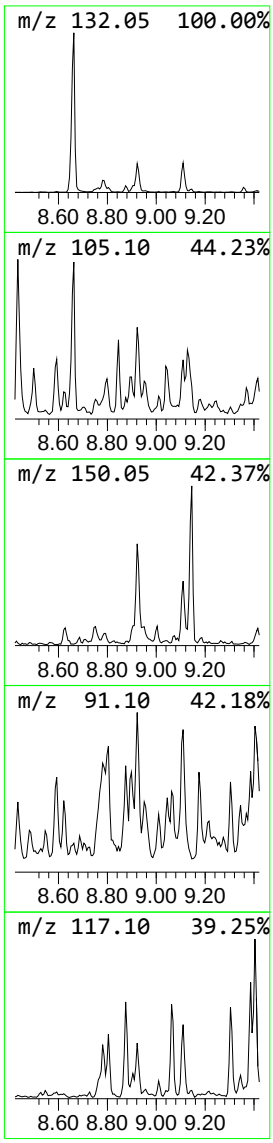
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 2,4,6-Trimethylbenzyl alcohol Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.922	7.05 ng	329338	Naphthalene-d8	8.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,6-Trimethylbenzyl alcohol	150	C10H14O	1000342-65-8	93
2	Benzenemethanol, 2,4,5-trimethyl-	150	C10H14O	004393-05-9	53
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	41
4	(3R)-1,2,3,4-Tetrahydro-3-isoqui...	163	C10H13NO	062855-02-1	38
5	Benzene, 4-ethenyl-1,2-dimethyl-	132	C10H12	027831-13-6	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
Data File : BF137341.D
Acq On : 08 Feb 2024 16:52
Operator : CG\JU
Sample : P1342-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323P-GW-20240131-0

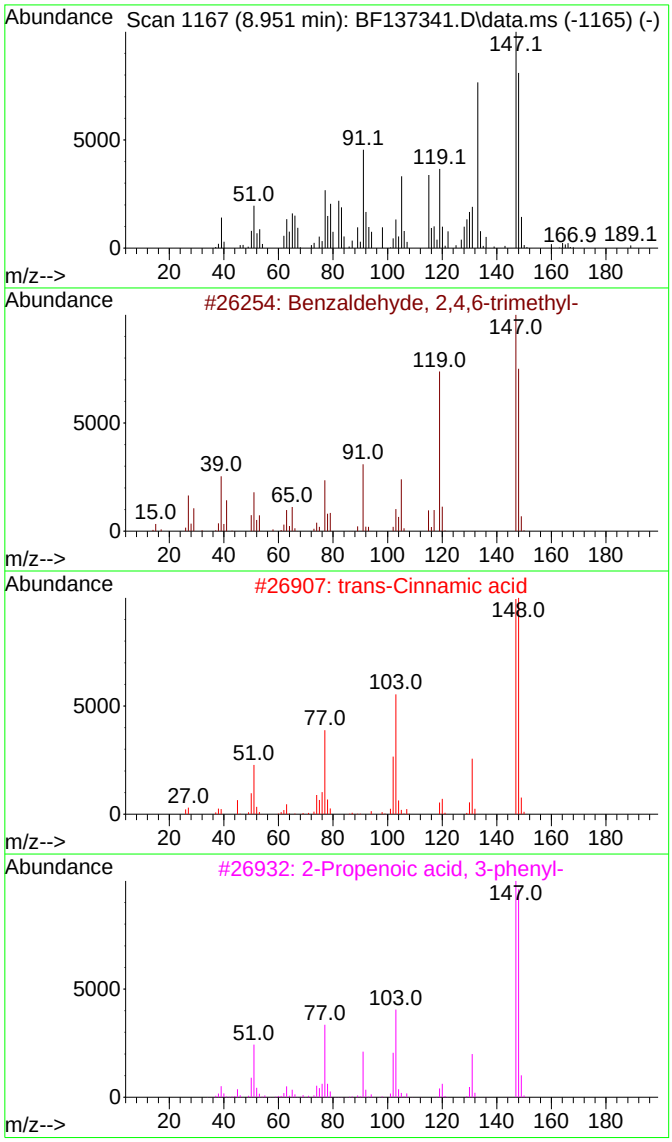
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

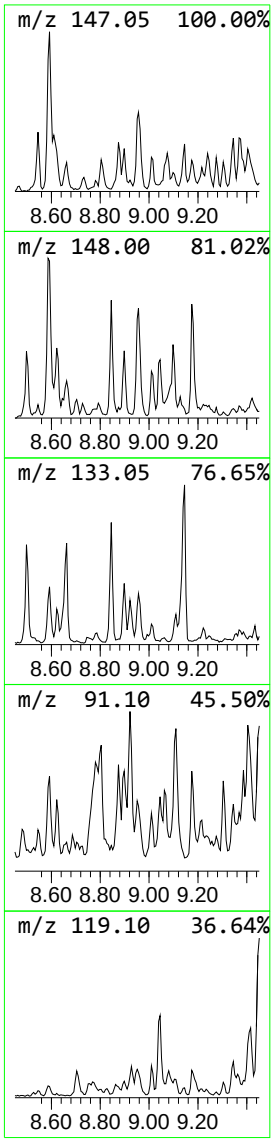
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 Benzaldehyde, 2,4,6-trimethyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.951	6.59 ng	344000	Acenaphthene-d10	9.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 2,4,6-trimethyl-	148	C10H12O	000487-68-3	64
2	trans-Cinnamic acid	148	C9H8O2	000140-10-3	60
3	2-Propenoic acid, 3-phenyl-	148	C9H8O2	000621-82-9	60
4	Benzaldehyde, 4-(1-methylethyl)-	148	C10H12O	000122-03-2	55
5	Benzaldehyde, 2,4,5-trimethyl-	148	C10H12O	005779-72-6	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
Data File : BF137341.D
Acq On : 08 Feb 2024 16:52
Operator : CG\JU
Sample : P1342-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323P-GW-20240131-0

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

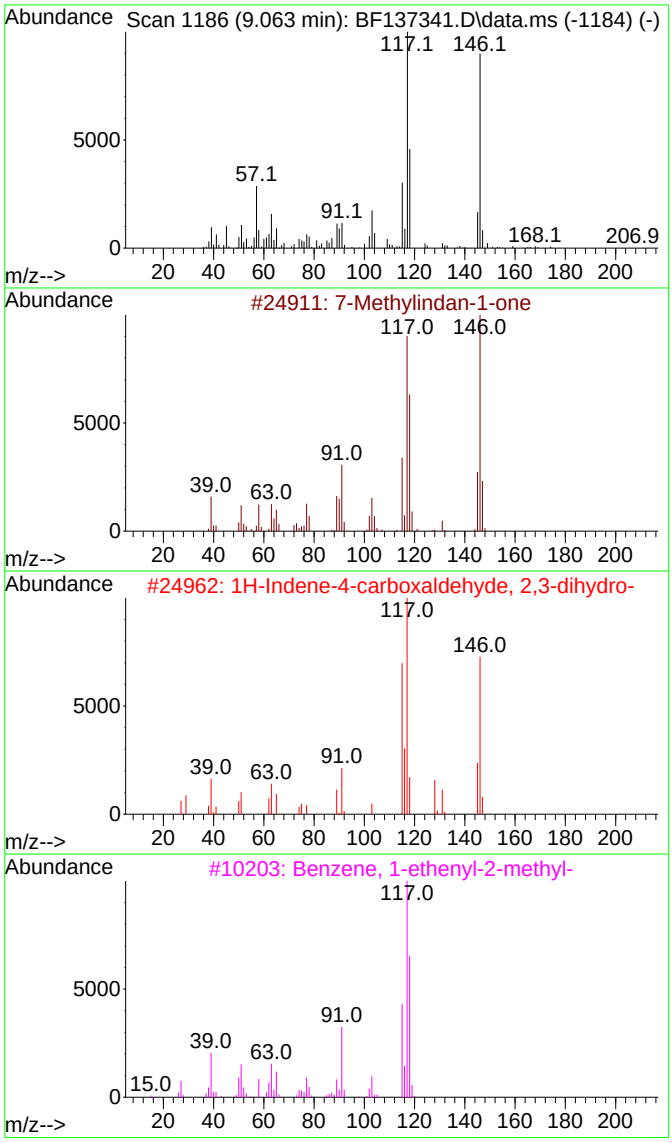
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

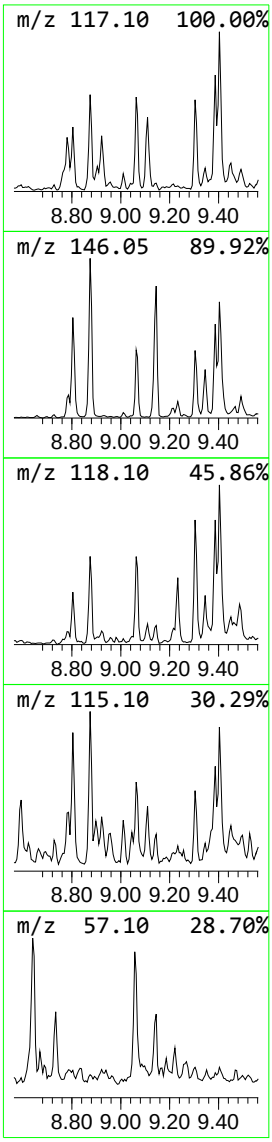
****

Peak Number 14 7-Methylindan-1-one Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.063	5.38 ng	280541	Acenaphthene-d10	9.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Methylindan-1-one	146	C10H10O	039627-61-7	74
2	1H-Indene-4-carboxaldehyde, 2,3-...	146	C10H10O	051932-70-8	58
3	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	50
4	2(1H)-Quinazolinone	146	C8H6N2O	007471-58-1	46
5	4H-1-Benzopyran-4-one	146	C9H6O2	000491-38-3	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
Data File : BF137341.D
Acq On : 08 Feb 2024 16:52
Operator : CG\JU
Sample : P1342-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323P-GW-20240131-0

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

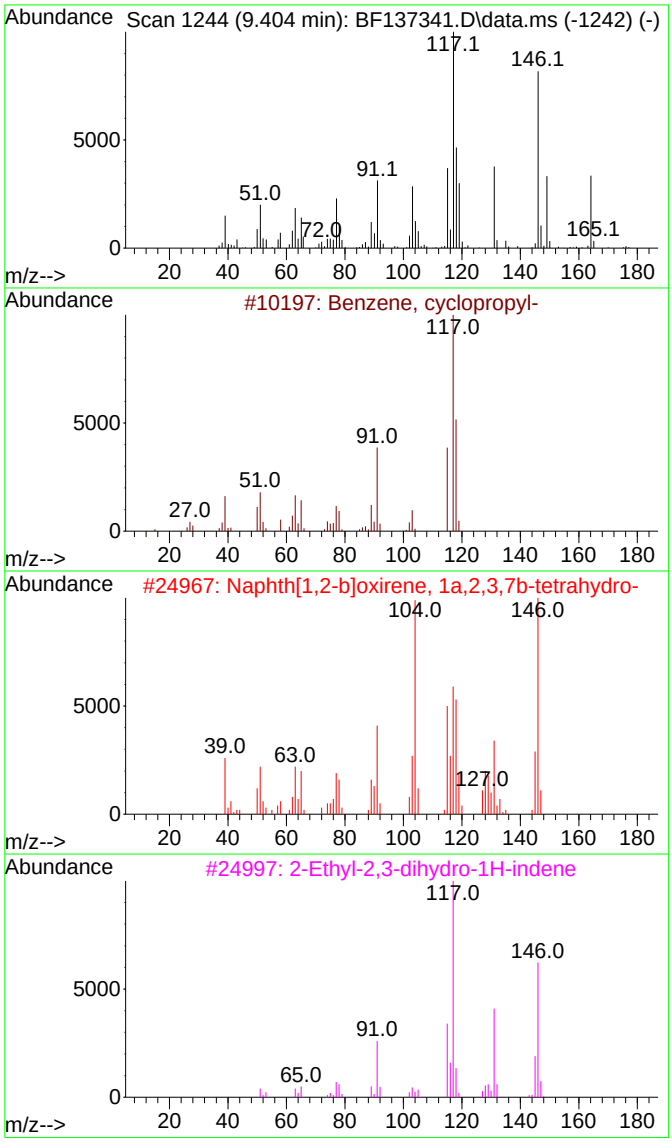
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

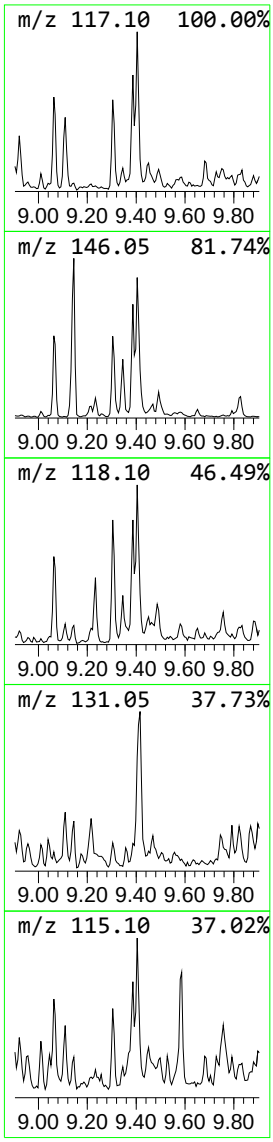
****

Peak Number 15 Benzene, cyclopropyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.404	10.45 ng	545430	Acenaphthene-d10	9.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, cyclopropyl-	118	C9H10	000873-49-4	83
2	Naphth[1,2-b]oxirene, 1a,2,3,7b-...	146	C10H10O	002461-34-9	58
3	2-Ethyl-2,3-dihydro-1H-indene	146	C11H14	056147-63-8	52
4	1H-Imidazole, 4,5-dihydro-2-phenyl-	146	C9H10N2	000936-49-2	49
5	2,3,4,5,6,7-Hexahydro-1H-cyclope...	146	C11H14	1010189-31-0	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
Data File : BF137341.D
Acq On : 08 Feb 2024 16:52
Operator : CG\JU
Sample : P1342-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323P-GW-20240131-0

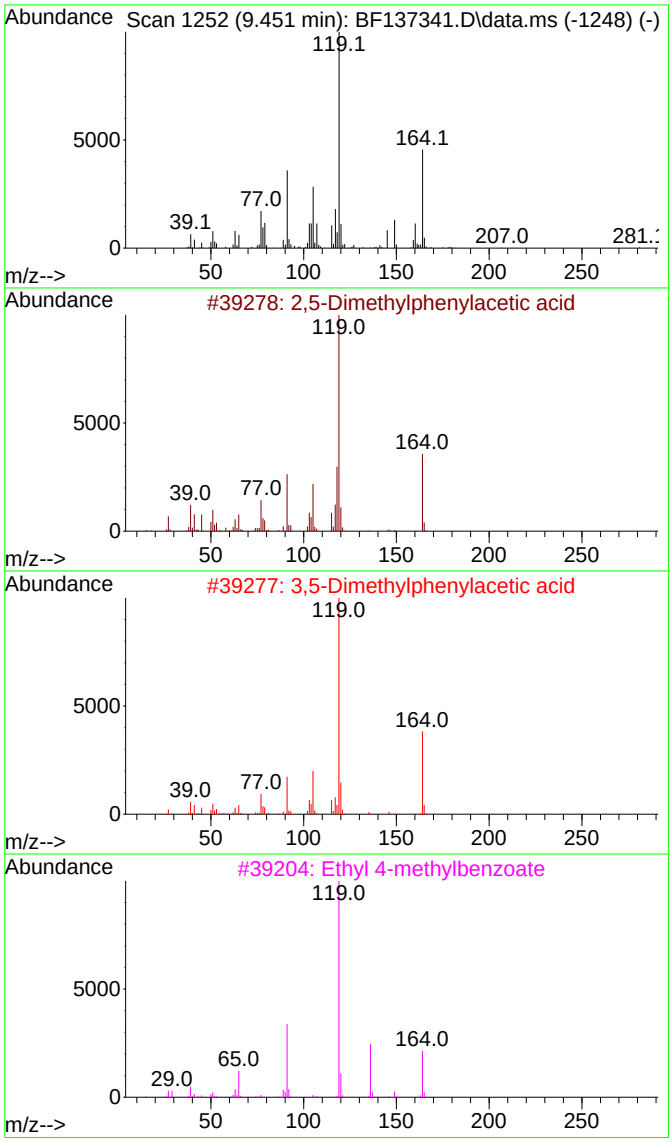
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

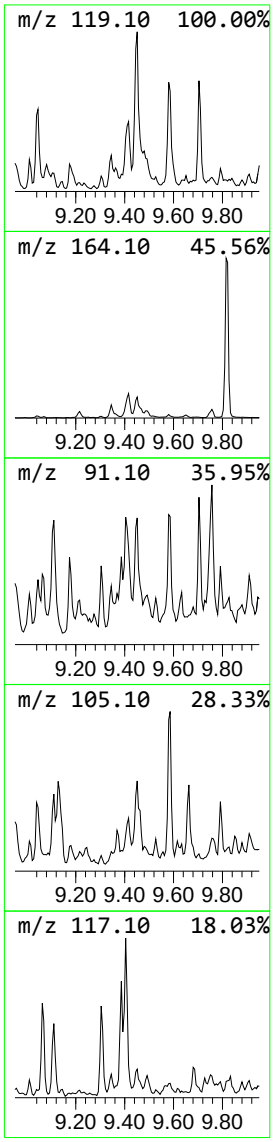
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 16 2,5-Dimethylphenylacetic acid Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.451	5.34 ng	278709	Acenaphthene-d10	9.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Dimethylphenylacetic acid	164	C10H12O2	1000342-65-5	87
2	3,5-Dimethylphenylacetic acid	164	C10H12O2	042288-46-0	81
3	Ethyl 4-methylbenzoate	164	C10H12O2	000094-08-6	52
4	Ethyl o-methylbenzoate	164	C10H12O2	000087-24-1	49
5	Benzene, 1-ethyl-4-(2-methylprop...	162	C12H18	100319-40-2	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
Data File : BF137341.D
Acq On : 08 Feb 2024 16:52
Operator : CG\JU
Sample : P1342-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323P-GW-20240131-0

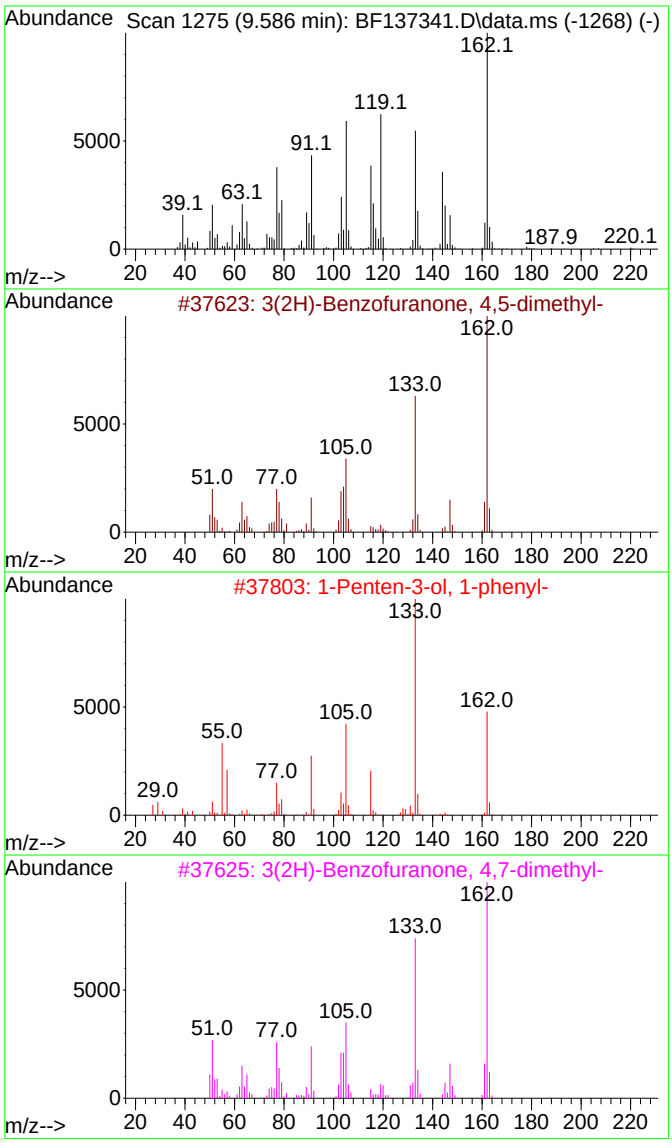
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

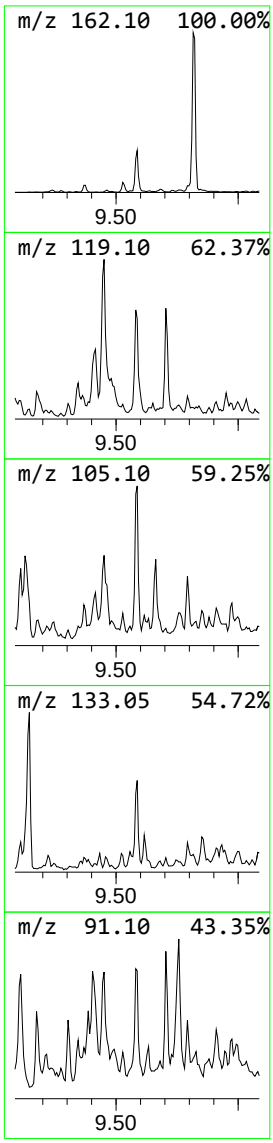
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 17 3(2H)-Benzofuranone, 4,5-di... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.586	11.71 ng	611060	Acenaphthene-d10	9.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3(2H)-Benzofuranone, 4,5-dimethyl-	162	C10H10O2	020895-42-5	50
2	1-Penten-3-ol, 1-phenyl-	162	C11H14O	034862-94-7	43
3	3(2H)-Benzofuranone, 4,7-dimethyl-	162	C10H10O2	020895-45-8	43
4	6-Methoxy-1-indanone	162	C10H10O2	013623-25-1	42
5	2-methyl-3-azabicyclo[3.2.1]octa...	162	C10H14N2	1000451-79-1	41





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
Data File : BF137341.D
Acq On : 08 Feb 2024 16:52
Operator : CG\JU
Sample : P1342-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323P-GW-20240131-0

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

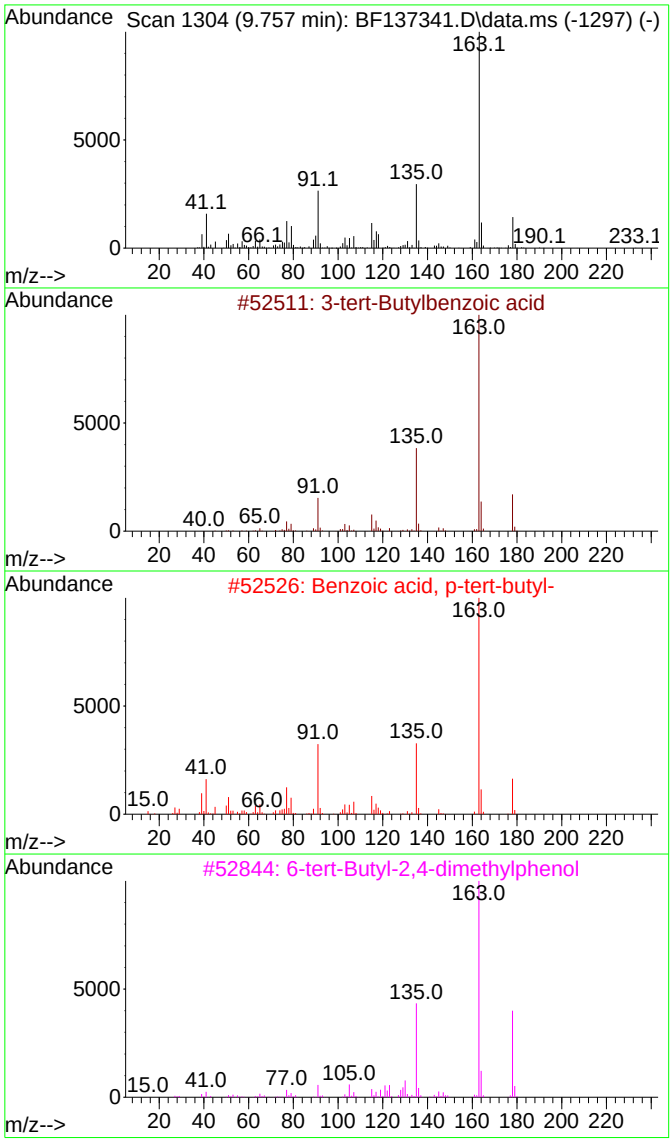
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

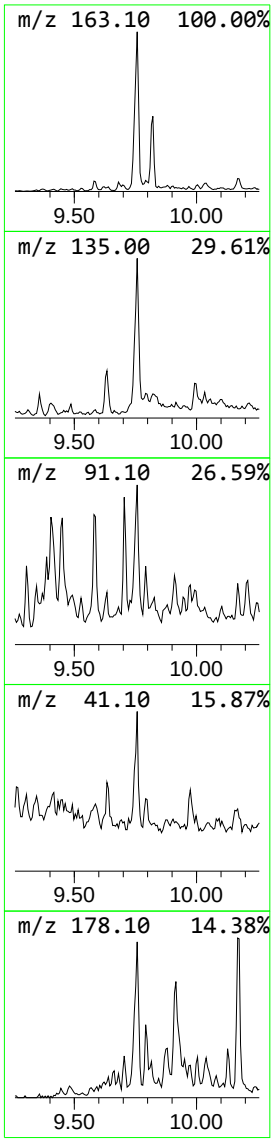
****

Peak Number 18 3-tert-Butylbenzoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.757	10.40 ng	542715	Acenaphthene-d10	9.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-tert-Butylbenzoic acid	178	C11H14O2	007498-54-6	90
2	Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	87
3	6-tert-Butyl-2,4-dimethylphenol	178	C12H18O	001879-09-0	74
4	Benzoic acid, 4-acetyl-, methyl ...	178	C10H10O3	003609-53-8	72
5	4-tert-Butyl-2,6-dimethylphenol	178	C12H18O	000879-97-0	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
Data File : BF137341.D
Acq On : 08 Feb 2024 16:52
Operator : CG\JU
Sample : P1342-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323P-GW-20240131-0

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

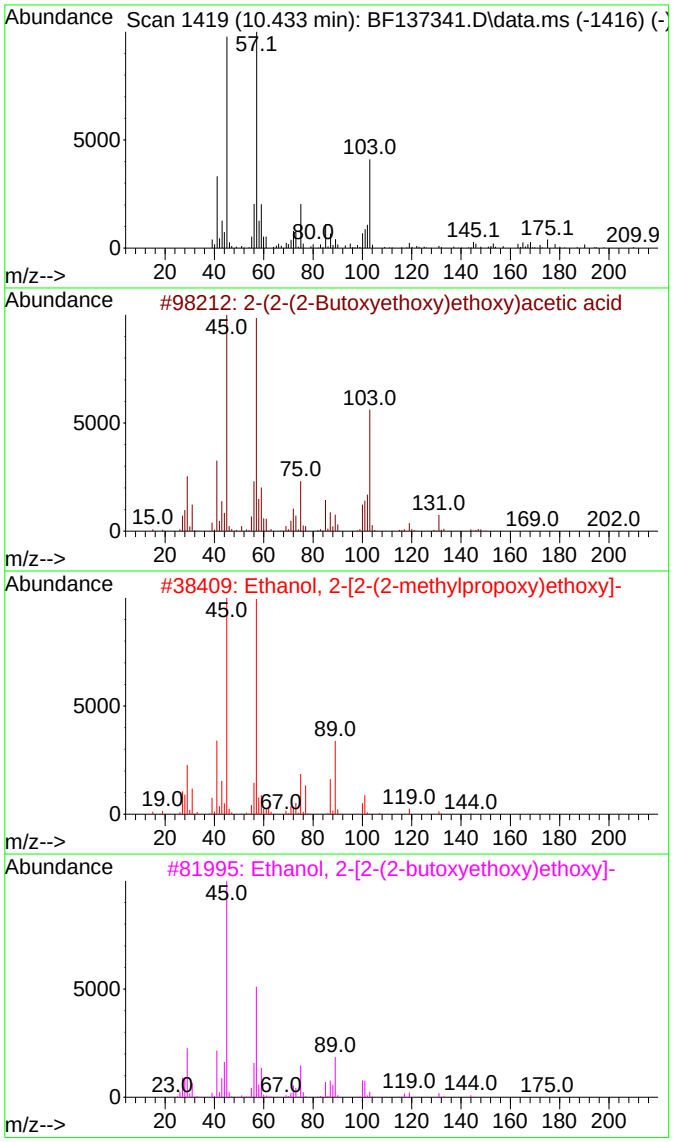
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

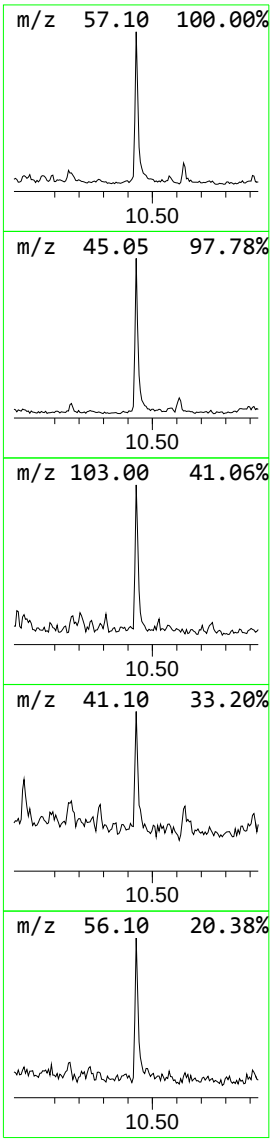
****

Peak Number 19 unknown10.433 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.433	5.46 ng	284974	Acenaphthene-d10	9.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(2-(2-Butoxyethoxy)ethoxy)acet...	220	C10H20O5	075427-76-8	49
2	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	47
3	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	47
4	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	47
5	Orthoformic acid, tri-sec-butyl ...	232	C13H28O3	016754-48-6	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
Data File : BF137341.D
Acq On : 08 Feb 2024 16:52
Operator : CG\JU
Sample : P1342-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323P-GW-20240131-0

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

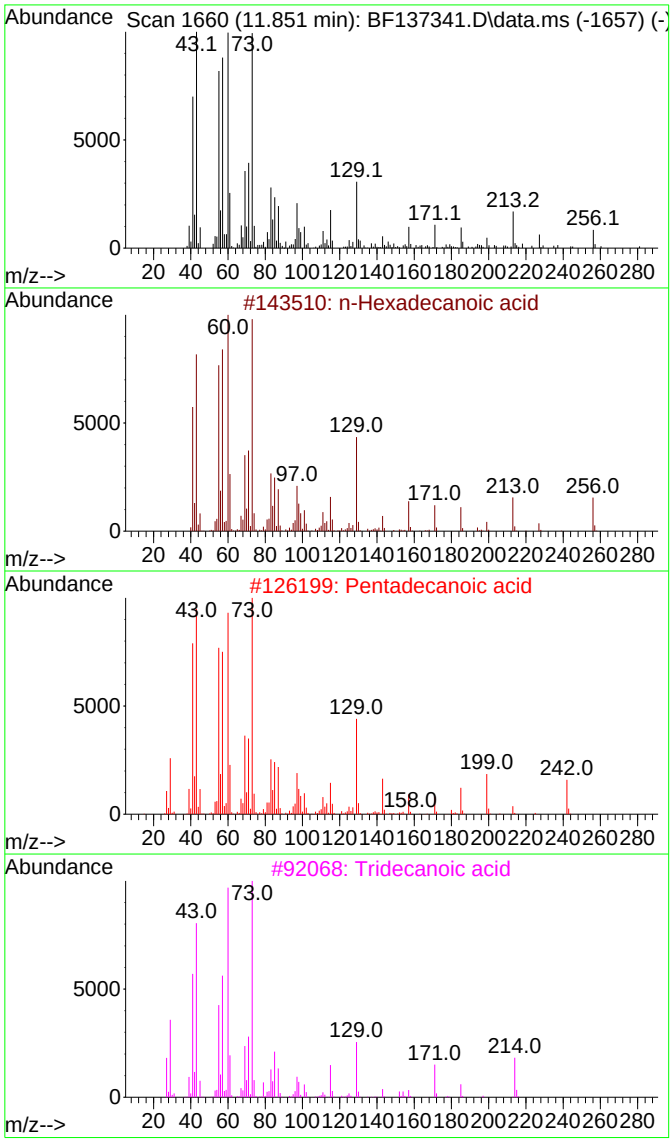
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

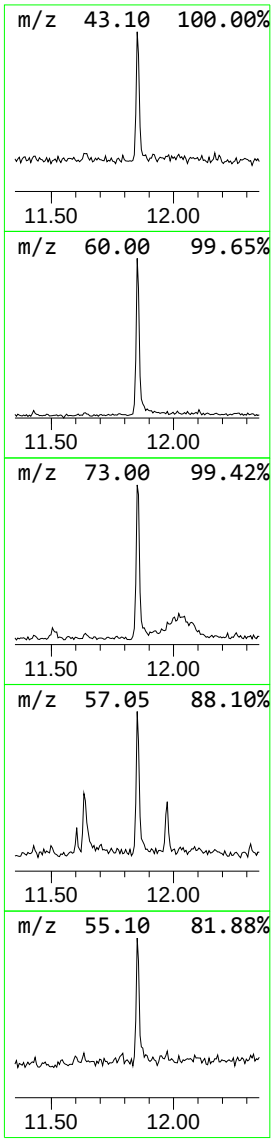
****

Peak Number 20 n-Hexadecanoic acid Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.851	5.98 ng	253021	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5	Undecanoic acid	186	C11H22O2	000112-37-8	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
Data File : BF137341.D
Acq On : 08 Feb 2024 16:52
Operator : CG\JU
Sample : P1342-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-323P-GW-20240131-0

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-...	3.122	15.4	ng	580507	1	6.781	754759	20.0
unknown7.033	7.033	9.6	ng	360511	1	6.781	754759	20.0
unknown7.110	7.110	7.2	ng	272740	1	6.781	754759	20.0
unknown7.633	7.633	8.7	ng	404906	2	8.063	934737	20.0
unknown8.186	8.186	6.2	ng	291159	2	8.063	934737	20.0
unknown8.292	8.292	9.4	ng	438835	2	8.063	934737	20.0
1H-Inden-5-ol, ...	8.333	33.2	ng	1549950	2	8.063	934737	20.0
unknown8.592	8.592	7.8	ng	363950	2	8.063	934737	20.0
1H-Inden-1-one,...	8.663	40.1	ng	1876210	2	8.063	934737	20.0
1H-Inden-1-one,...	8.804	7.8	ng	364408	2	8.063	934737	20.0
1-Methylindan-2...	8.875	12.1	ng	565866	2	8.063	934737	20.0
2,4,6-Trimethyl...	8.922	7.0	ng	329338	2	8.063	934737	20.0
Benzaldehyde, 2...	8.951	6.6	ng	344000	3	9.816	1043810	20.0
7-Methylindan-1...	9.063	5.4	ng	280541	3	9.816	1043810	20.0
Benzene, cyclop...	9.404	10.4	ng	545430	3	9.816	1043810	20.0
2,5-Dimethylphe...	9.451	5.3	ng	278709	3	9.816	1043810	20.0
3(2H)-Benzofura...	9.586	11.7	ng	611060	3	9.816	1043810	20.0
3-tert-Butylben...	9.757	10.4	ng	542715	3	9.816	1043810	20.0
unknown10.433	10.433	5.5	ng	284974	3	9.816	1043810	20.0
n-Hexadecanoic ...	11.851	6.0	ng	253021	4	11.310	846180	20.0