LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110922\
Data File : BF131100.D
Acq On : 09 Nov 2022 22:06
Operator : CG\JU
Sample : N5340-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

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-BF110922.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131100.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	6	12	rBV	189003	214763	2.89%	0.234%
2	2.193	12	18	25	rVB	1650571	2181390	29.36%	2.376%
3	2.322	31	40	49	rVB2	100307	201524	2.71%	0.219%
4	3.422	220	227	234	rBV	156715	270933	3.65%	0.295%
5	5.116	510	515	520	rBV	396472	433101	5.83%	0.472%
6	5.510	579	582	585	rBV	904472	991907	13.35%	1.080%
7	5.728	615	619	626	rVV3	545329	695988	9.37%	0.758%
8	6.363	722	727	732	rVB3	150710	253594	3.41%	0.276%
9	6.469	743	745	747	rBV	288647	220305	2.97%	0.240%
10	6.528	750	755	760	rBV2	469104	821481	11.06%	0.895%
11	6.710	783	786	789	rBV	221333	205293	2.76%	0.224%
12	6.893	813	817	820	rBV	679818	622939	8.39%	0.678%
13	6.951	820	827	828	rBV2	696110	774344	10.42%	0.843%
14	6.969	828	830	837	rVV	736353	1041390	14.02%	1.134%
15	7.051	840	844	855	rVB	1581399	2596741	34.96%	2.828%
16	7.145	858	860	863	rBV	241122	273422	3.68%	0.298%
17	7.298	879	886	889	rVV	616711	892436	12.01%	0.972%
18	7.375	892	899	902	rVV2	466901	901276	12.13%	0.982%
19	7.422	903	907	908	rVV2	257291	307043	4.13%	0.334%
20	7.463	908	914	916	rVV2	1982879	2620563	35.28%	2.854%
21	7.492	916	919	924	rVB2	1318547	1301205	17.52%	1.417%
22	7.645	935	945	946	rBV3	337899	698317	9.40%	0.761%
23	7.722	950	958	959	rVV	550973	1020905	13.74%	1.112%
24	7.781	965	968	969	rBV	195918	229564	3.09%	0.250%
25	7.898	973	988	991	rVV3	1582585	5077009	68.34%	5.529%
26	7.928	991	993	996	rVB	2320517	1914844	25.78%	2.085%
27	7.987	998	1003	1007	rBV4	532849	880436	11.85%	0.959%
28	8.045	1008	1013	1014	rBV4	319382	464728	6.26%	0.506%
29	8.104	1020	1023	1028	rBV2	901368	1833781	24.68%	1.997%
30	8.181	1033	1036	1037	rVV	1274534	1487110	20.02%	1.620%
31	8.198	1037	1039	1040	rVV	1688186	1305003	17.57%	1.421%
32	8.216	1040	1042	1045	rVB	3561420	3094859	41.66%	3.370%
33	8.316	1056	1059	1061	rBV3	184993	185011	2.49%	0.201%
34	8.345	1061	1064	1066	rVB2	714158	624494	8.41%	0.680%
35	8.381	1066	1070	1071	rBV2	201555	230849	3.11%	0.251%
36	8.398	1071	1073	1077	rBV3	383844	411522	5.54%	0.448%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110922\
Data File : BF131100.D
Acq On : 09 Nov 2022 22:06
Operator : CG\JU
Sample : N5340-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

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-BF110922.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	8.434	1077	1079	1083	rVB4	250605	250703	3.37%	0.273%
38	8.469	1083	1085	1088	rVB3	256697	214324	2.89%	0.233%
39	8.545	1091	1098	1100	rBV2	823256	1380772	18.59%	1.504%
40	8.604	1104	1108	1110	rBV2	663731	759182	10.22%	0.827%
41	8.628	1110	1112	1113	rBV	358864	252776	3.40%	0.275%
42	8.639	1113	1114	1116	rVB	657378	446708	6.01%	0.486%
43	8.687	1119	1122	1126	rVB3	791604	1078005	14.51%	1.174%
44	8.739	1126	1131	1138	rBV5	974107	1800671	24.24%	1.961%
45	8.798	1138	1141	1144	rBV3	343885	356974	4.81%	0.389%
46	8.851	1148	1150	1154	rVB4	272842	354364	4.77%	0.386%
47	8.892	1154	1157	1161	rBV3	345461	454440	6.12%	0.495%
48	8.928	1161	1163	1168	rBV4	351032	447788	6.03%	0.488%
49	8.969	1168	1170	1172	rVB	330714	212529	2.86%	0.231%
50	9.016	1175	1178	1181	rVB	302463	328091	4.42%	0.357%
51	9.051	1181	1184	1186	rBV2	279836	305462	4.11%	0.333%
52	9.104	1187	1193	1195	rBV5	331140	492023	6.62%	0.536%
53	9.145	1197	1200	1203	rBV2	425576	520509	7.01%	0.567%
54	9.175	1203	1205	1209	rVB4	389258	455860	6.14%	0.496%
55	9.257	1209	1219	1222	rVB	4004813	4874468	65.62%	5.309%
56	9.298	1222	1226	1229	rBV3	286207	429419	5.78%	0.468%
57	9.334	1229	1232	1234	rBV2	440163	363111	4.89%	0.395%
58	9.363	1234	1237	1239	rBV2	371243	435830	5.87%	0.475%
59	9.439	1239	1250	1252	rVB	3926973	7428776	100.00%	8.090%
60	9.469	1252	1255	1259	rBV2	535154	515420	6.94%	0.561%
61	9.592	1274	1276	1278	rBV	273351	234160	3.15%	0.255%
62	9.622	1278	1281	1284	rVB5	336468	457553	6.16%	0.498%
63	9.704	1289	1295	1302	rVB2	902421	1385745	18.65%	1.509%
64	9.763	1302	1305	1307	rBV3	281239	265613	3.58%	0.289%
65	9.816	1307	1314	1317	rVB5	541683	723030	9.73%	0.787%
66	9.886	1317	1326	1328	rBV	2811752	3613341	48.64%	3.935%
67	9.939	1332	1335	1337	rVB	832768	605606	8.15%	0.660%
68	9.986	1337	1343	1345	rBV5	296247	450745	6.07%	0.491%
69	10.051	1351	1354	1357	rBV3	181669	306635	4.13%	0.334%
70	10.086	1357	1360	1364	rVV4	243625	380770	5.13%	0.415%
71	10.169	1372	1374	1377	rBV2	319835	265304	3.57%	0.289%
72	10.228	1381	1384	1386	rBV	415110	499874	6.73%	0.544%
73	10.292	1386	1395	1398	rVB	2065280	4917361	66.19%	5.355%
74	10.463	1419	1424	1425	rBV3	244546	357833	4.82%	0.390%
75	10.528	1432	1435	1437	rBV3	215269	252782	3.40%	0.275%
76	10.604	1445	1448	1451	rVB	630520	579093	7.80%	0.631%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110922\
Data File : BF131100.D
Acq On : 09 Nov 2022 22:06
Operator : CG\JU
Sample : N5340-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

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-BF110922.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	10.710	1462	1466	1467	rBV2	405684	429514	5.78%	0.468%
78	10.739	1467	1471	1473	rVV	1894534	1739556	23.42%	1.894%
79	10.769	1473	1476	1479	rVB4	387409	364019	4.90%	0.396%
80	10.881	1492	1495	1496	rBV	200712	184780	2.49%	0.201%
81	10.910	1496	1500	1504	rVB2	609264	665681	8.96%	0.725%
82	10.975	1508	1511	1517	rVB3	208288	315606	4.25%	0.344%
83	11.033	1518	1521	1525	rVB2	294924	352712	4.75%	0.384%
84	11.139	1535	1539	1542	rVB2	308660	331604	4.46%	0.361%
85	11.263	1558	1560	1563	rBV4	206616	238099	3.21%	0.259%
86	11.328	1566	1571	1574	rVB2	290174	385885	5.19%	0.420%
87	11.369	1574	1578	1580	rBV3	197514	298871	4.02%	0.325%
88	11.433	1585	1589	1591	rVB	752400	703534	9.47%	0.766%
89	11.775	1644	1647	1651	rBV3	166455	243775	3.28%	0.265%
90	11.957	1676	1678	1685	rVB2	226860	298847	4.02%	0.325%
91	12.057	1689	1695	1702	rVB2	1703574	2410931	32.45%	2.626%
92	12.180	1713	1716	1720	rVB2	155241	193346	2.60%	0.211%
93	12.410	1750	1755	1763	rVB2	726713	1044435	14.06%	1.137%
94	12.569	1779	1782	1785	rBV	559203	452141	6.09%	0.492%
95	12.739	1808	1811	1820	rVB2	357434	419930	5.65%	0.457%
96	13.022	1854	1859	1862	rVB	2532577	2411898	32.47%	2.627%
97	13.392	1919	1922	1927	rVB	215728	204875	2.76%	0.223%
98	14.074	2035	2038	2041	rVV	551256	469608	6.32%	0.511%
99	14.674	2137	2140	2148	rVB	339204	385113	5.18%	0.419%
100	15.568	2288	2292	2303	rVB	411380	543687	7.32%	0.592%

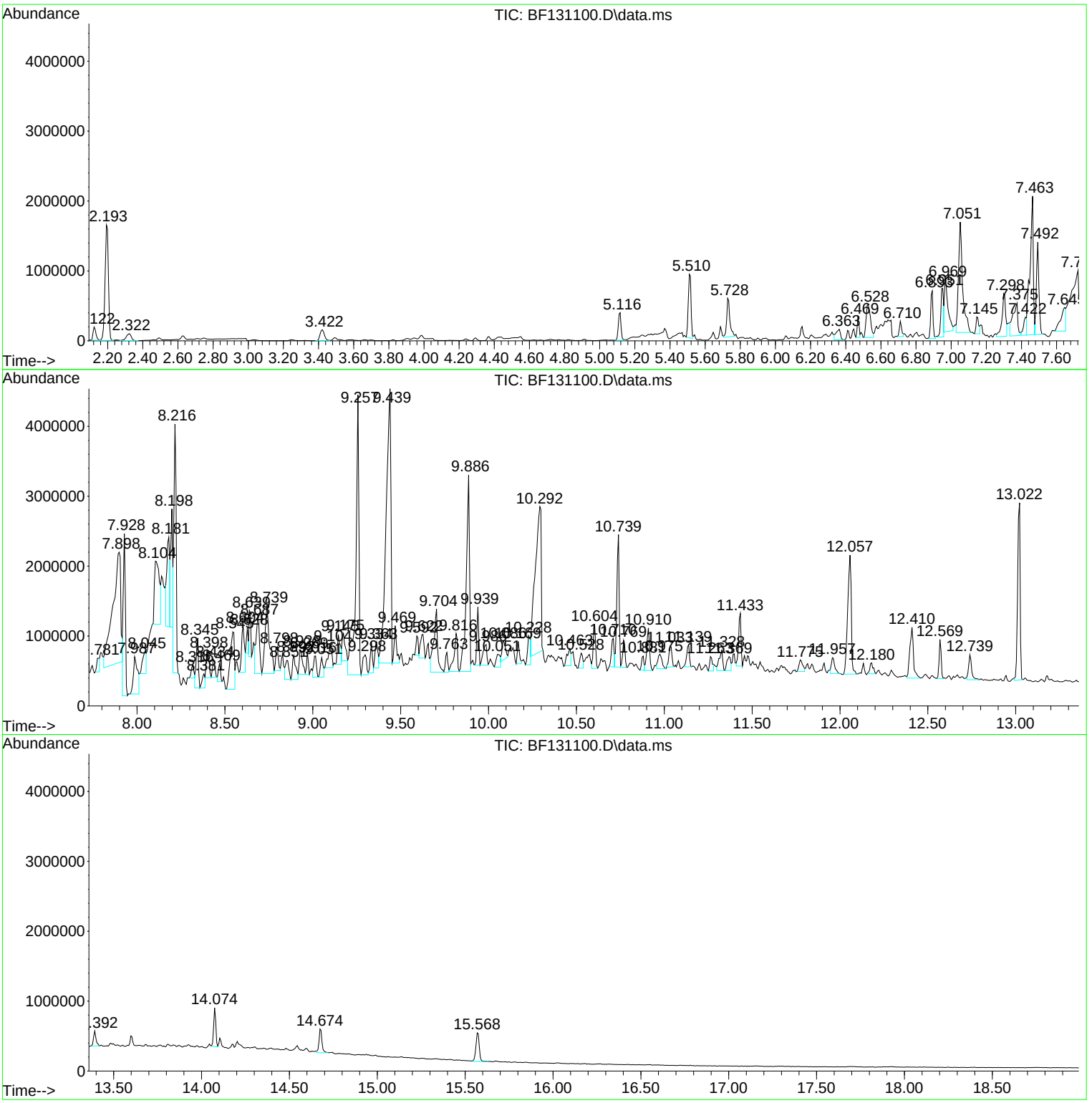
Sum of corrected areas: 91822167

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110922\
Data File : BF131100.D
Acq On : 09 Nov 2022 22:06
Operator : CG\JU
Sample : N5340-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.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\BF110922\
Data File : BF131100.D
Acq On : 09 Nov 2022 22:06
Operator : CG\JU
Sample : N5340-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

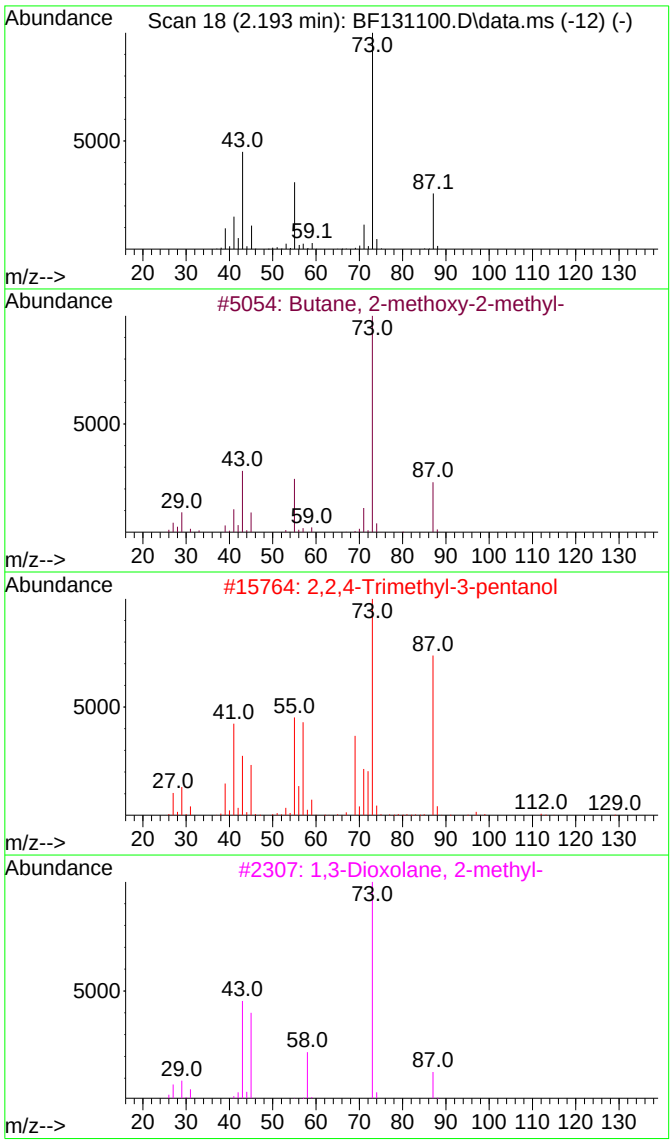
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

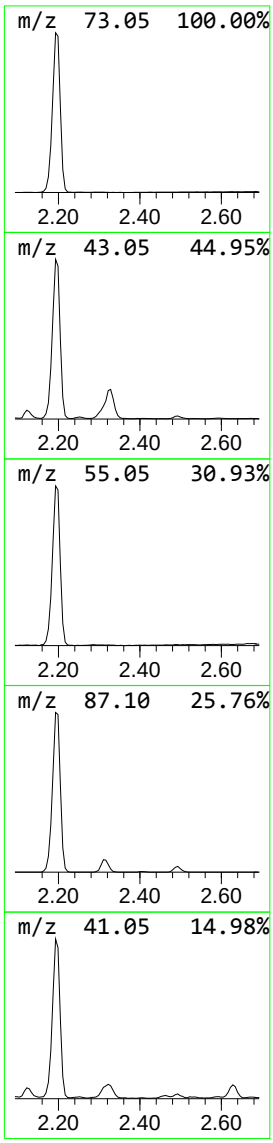
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.193	70.04 ng	2181390	1,4-Dichlorobenzene-d4	6.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110922\
Data File : BF131100.D
Acq On : 09 Nov 2022 22:06
Operator : CG\JU
Sample : N5340-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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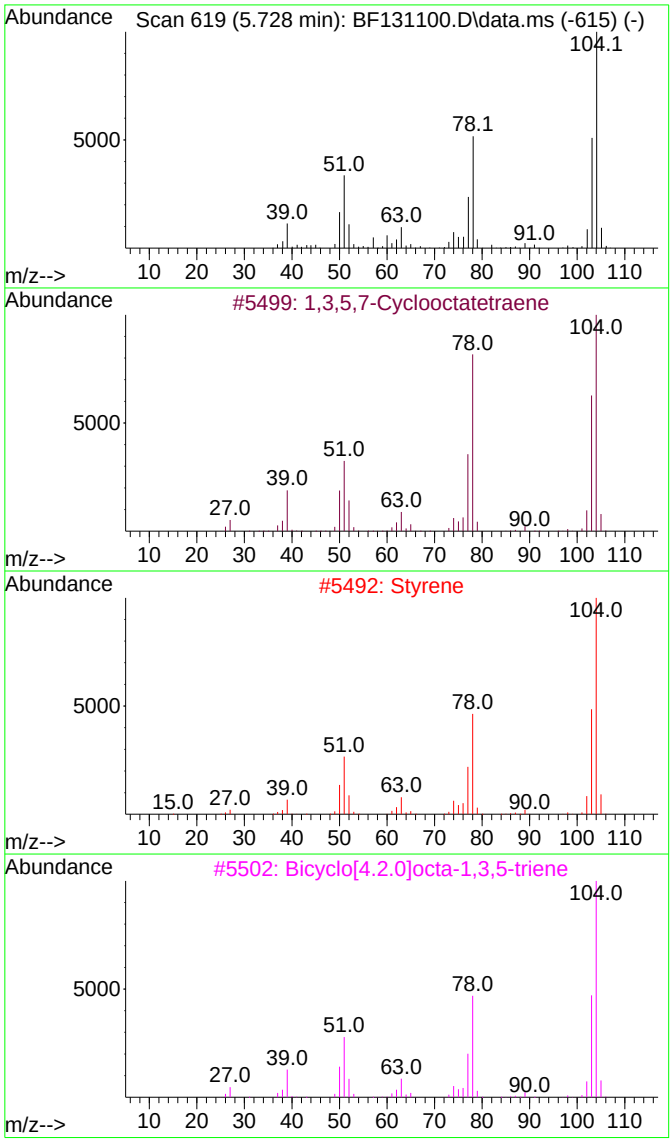
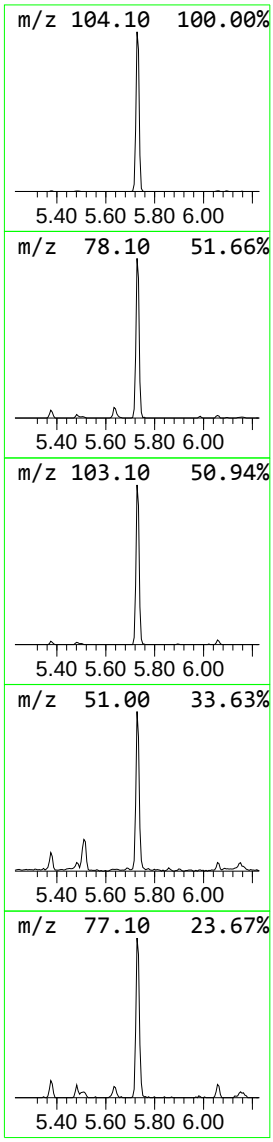
Peak Number 2 1,3,5,7-Cyclooctatetraene Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.728	22.35 ng	695988	1,4-Dichlorobenzene-d4	6.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5,7-Cyclooctatetraene	104	C8H8	000629-20-9	96
2	Styrene	104	C8H8	000100-42-5	96
3	Bicyclo[4.2.0]octa-1,3,5-triene	104	C8H8	000694-87-1	96
4	Butanedioic acid, phenyl-	194	C10H10O4	000635-51-8	64
5	1,3,7-Octatrien-5-yne	104	C8H8	016607-77-5	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110922\
Data File : BF131100.D
Acq On : 09 Nov 2022 22:06
Operator : CG\JU
Sample : N5340-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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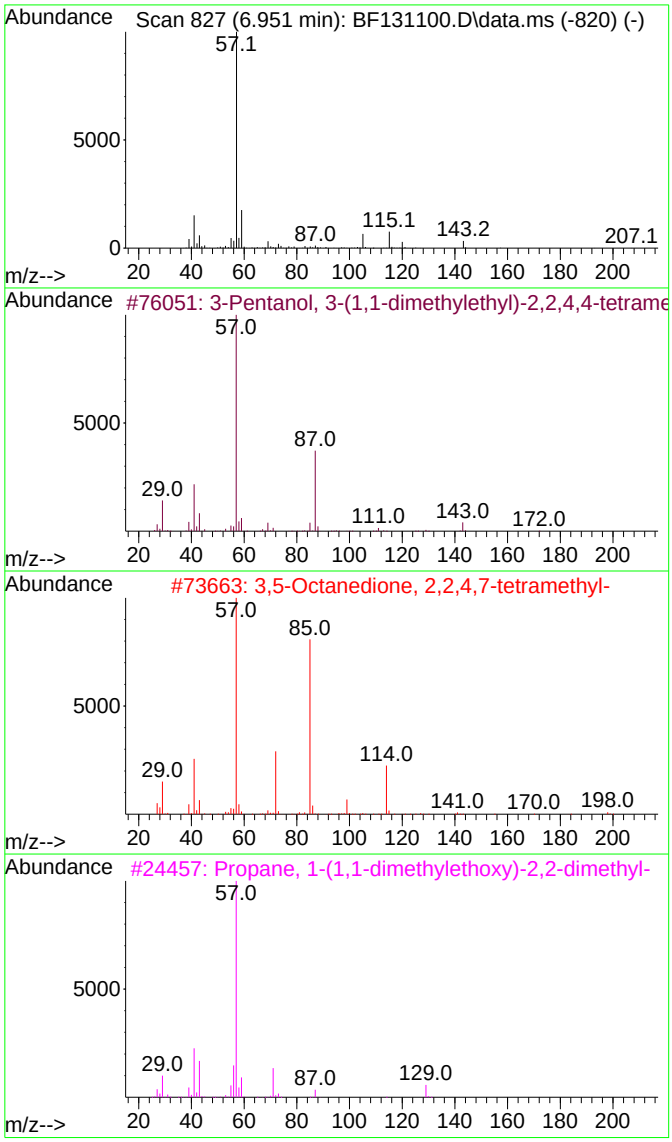
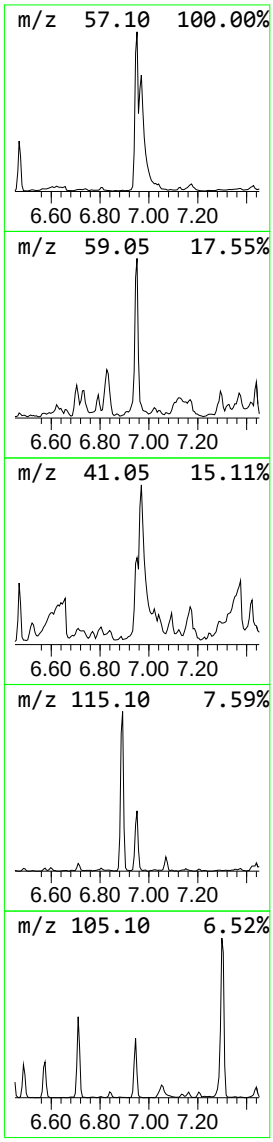
Peak Number 3 unknown6.951 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.951	24.86 ng	774344	1,4-Dichlorobenzene-d4	6.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanol, 3-(1,1-dimethylethyl...	200	C13H28O	041902-42-5	43
2	3,5-Octanedione, 2,2,4,7-tetrame...	198	C12H22O2	1000161-72-3	38
3	Propane, 1-(1,1-dimethylethoxy)-...	144	C9H20O	032970-46-0	28
4	Propanoic acid, 2,2-dimethyl-, t...	158	C9H18O2	016474-43-4	25
5	Ethanedioic acid, dibutyl ester	202	C10H18O4	002050-60-4	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110922\
Data File : BF131100.D
Acq On : 09 Nov 2022 22:06
Operator : CG\JU
Sample : N5340-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

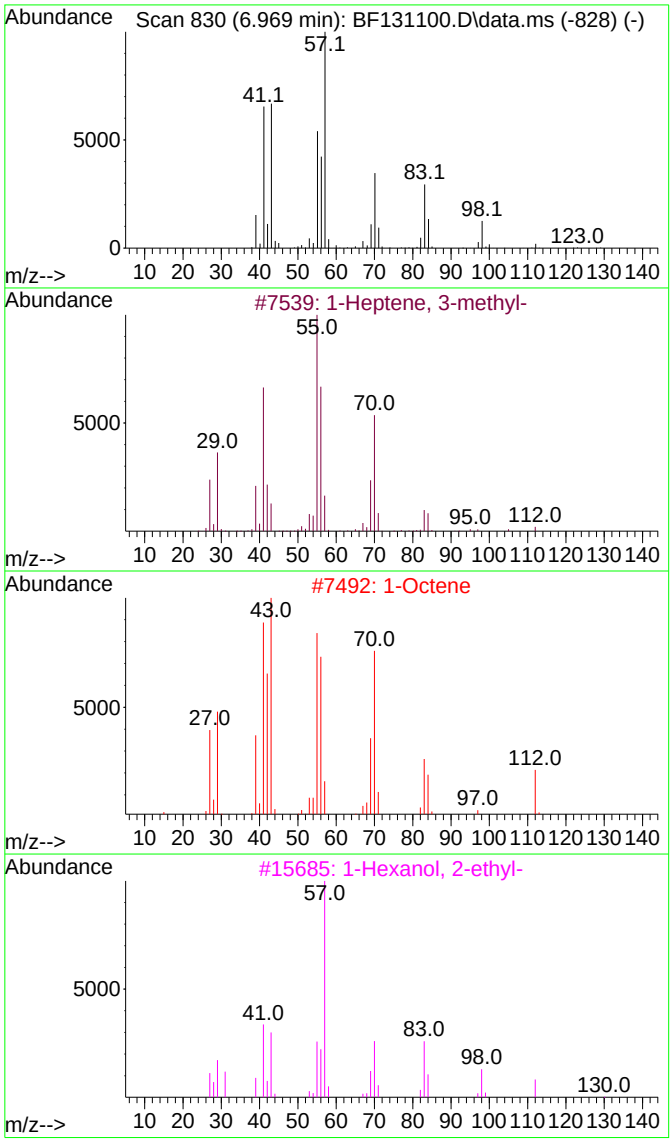
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

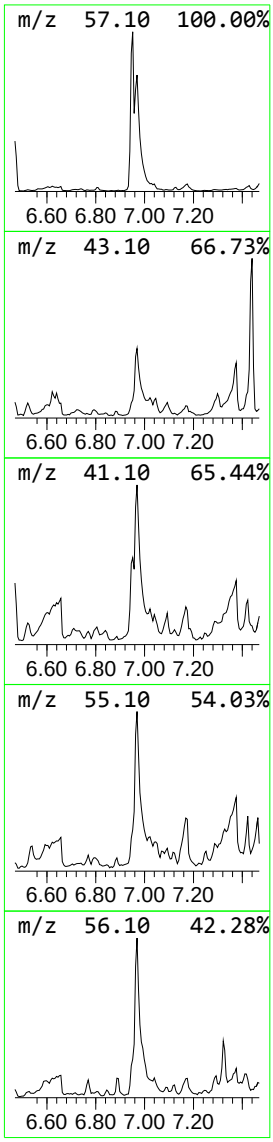
****

Peak Number 4 1-Heptene, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.969	33.43 ng	1041390	1,4-Dichlorobenzene-d4	6.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptene, 3-methyl-	112	C8H16	004810-09-7	52
2	1-Octene	112	C8H16	000111-66-0	50
3	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	50
4	Cycloheptane	98	C7H14	000291-64-5	50
5	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110922\
Data File : BF131100.D
Acq On : 09 Nov 2022 22:06
Operator : CG\JU
Sample : N5340-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

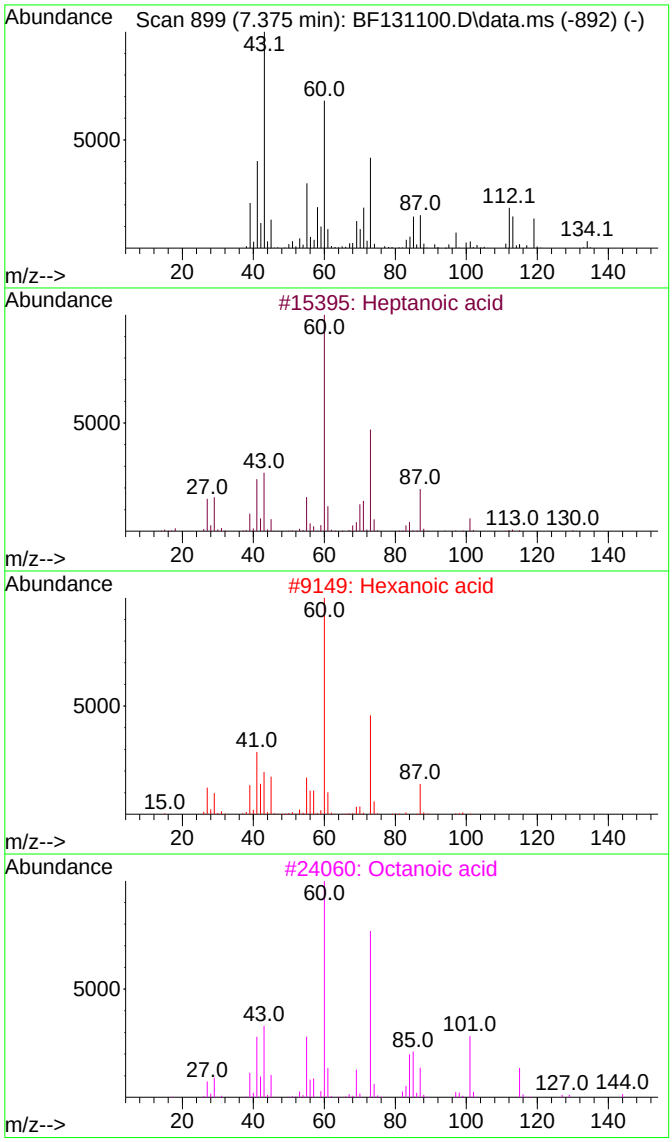
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

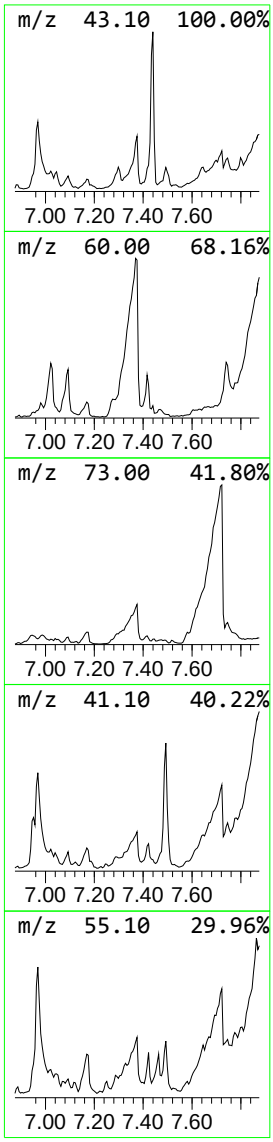
****

Peak Number 5 unknown7.375 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.375	28.94 ng	901276	1,4-Dichlorobenzene-d4	6.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanoic acid	130	C7H14O2	000111-14-8	38
2	Hexanoic acid	116	C6H12O2	000142-62-1	38
3	Octanoic acid	144	C8H16O2	000124-07-2	38
4	8-Chlorocapric acid	178	C8H15ClO2	001795-62-6	37
5	Pentanoic acid	102	C5H10O2	000109-52-4	37





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Acq On : 09 Nov 2022 22:06
Operator : CG\JU
Sample : N5340-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

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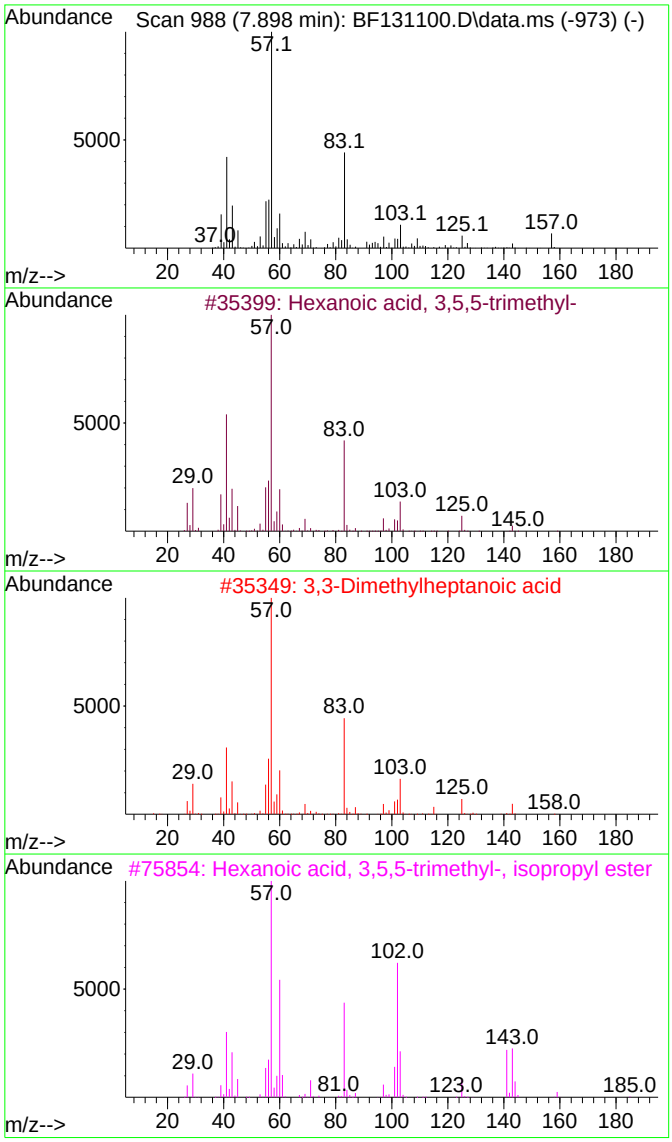
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

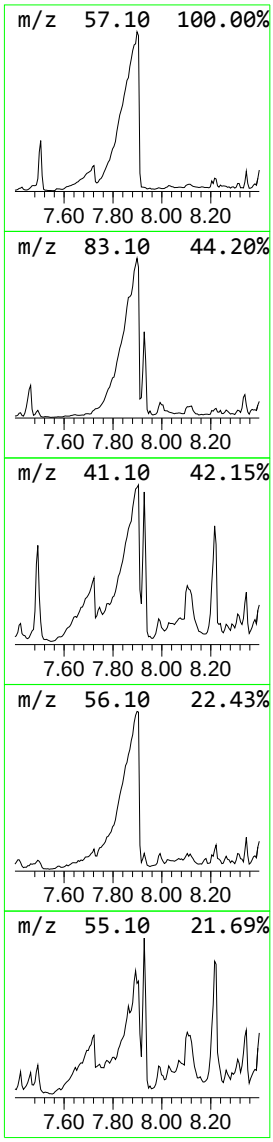
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Hexanoic acid, 3,5,5-trimet... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.898	68.28 ng	5077010	Naphthalene-d8	8.181

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	86
2	3,3-Dimethylheptanoic acid	158	C9H18O2	067061-30-7	64
3	Hexanoic acid, 3,5,5-trimethyl-,...	200	C12H24O2	1000406-05-1	42
4	Hexanoyl chloride, 3,5,5-trimethyl-	176	C9H17ClO	036727-29-4	40
5	Hexanal, 3,5,5-trimethyl-	142	C9H18O	005435-64-3	38





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ALS Vial : 9 Sample Multiplier: 1

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

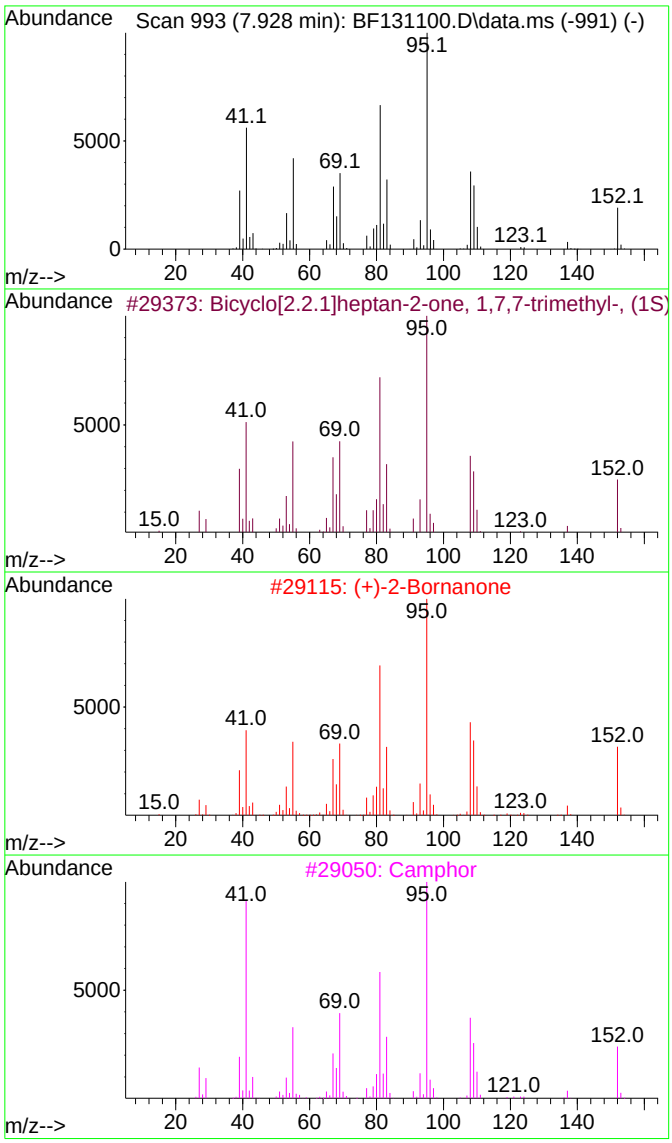
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

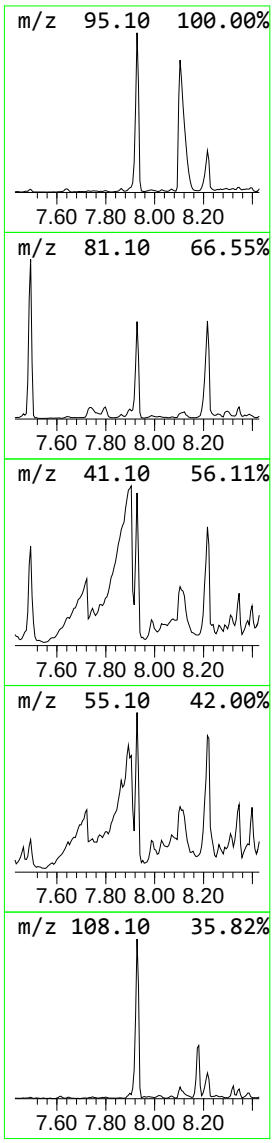
****

Peak Number 7 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.928	25.75 ng	1914840	Naphthalene-d8	8.181

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	98
2	(+)-2-Bornanone	152	C10H16O	000464-49-3	97
3	Camphor	152	C10H16O	000076-22-2	97
4	5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	006752-80-3	58
5	Bicyclo[3.1.0]hexane, 1,5-dimethyl-	110	C8H14	1010142-17-5	46





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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

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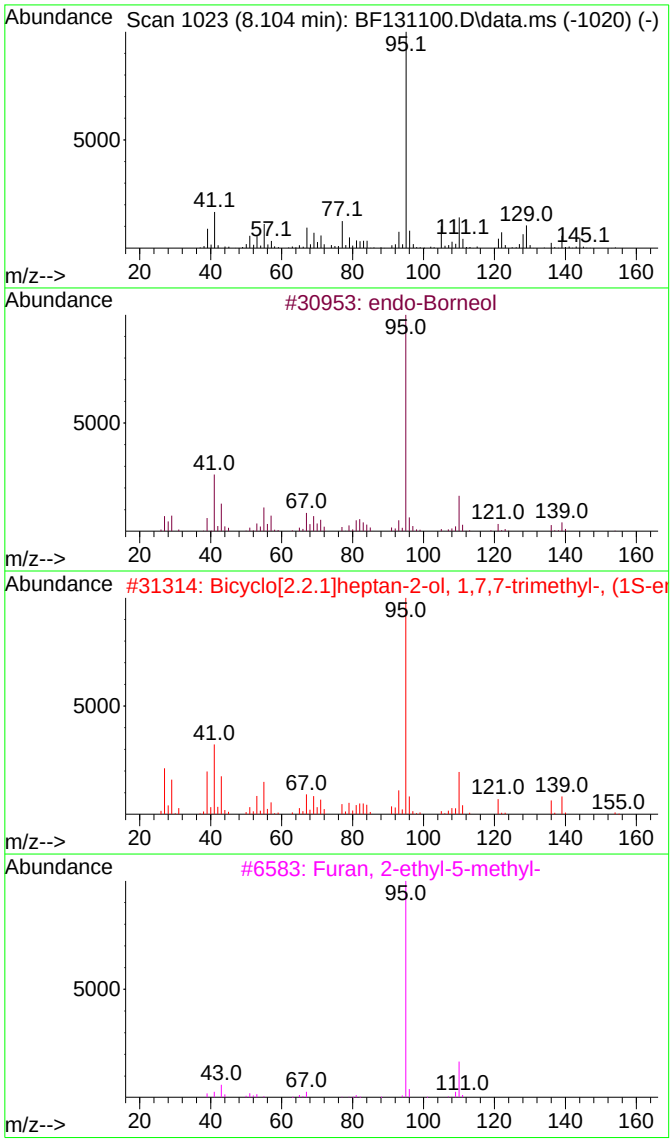
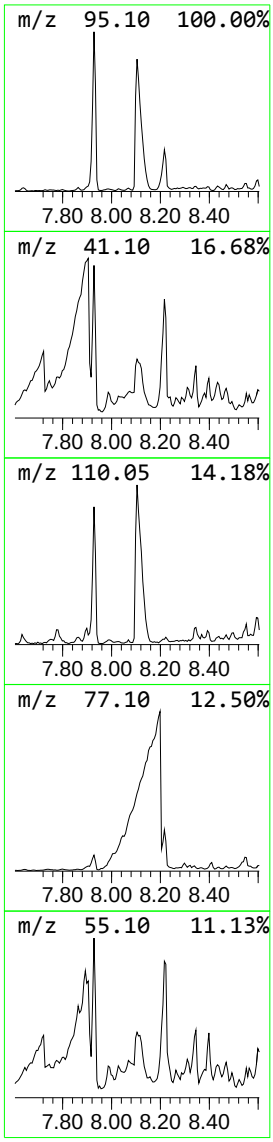
Peak Number 8 endo-Borneol Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.104	24.66 ng	1833780	Naphthalene-d8	8.181

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	endo-Borneol	154	C10H18O	000507-70-0	76
2	Bicyclo[2.2.1]heptan-2-ol, 1,7,7...	154	C10H18O	000464-45-9	53
3	Furan, 2-ethyl-5-methyl-	110	C7H10O	001703-52-2	52
4	Ethanone, 1-(2-furanyl)-	110	C6H6O2	001192-62-7	52
5	Bicyclo[3.1.0]hexane, 1,5-dimethyl-	110	C8H14	1010142-17-5	50





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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

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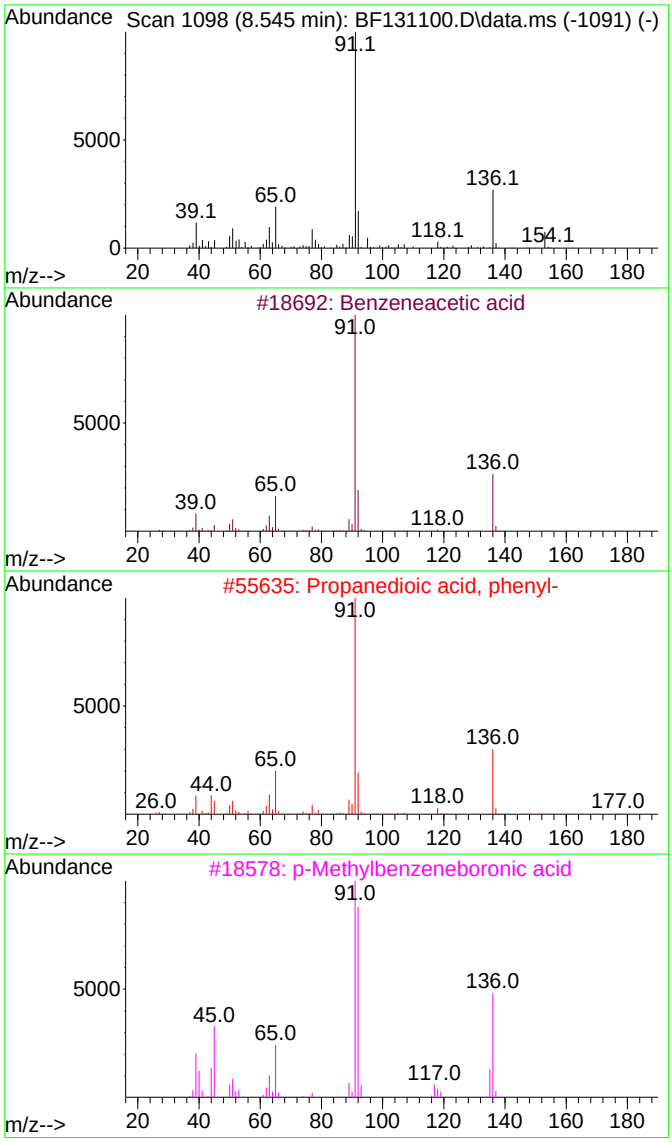
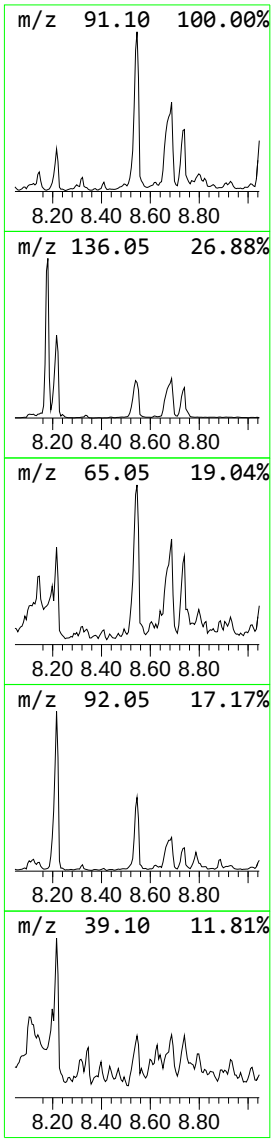
Peak Number 9 Benzeneacetic acid Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.545	18.57 ng	1380770	Naphthalene-d8	8.181

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzeneacetic acid	136	C8H8O2	000103-82-2	93
2	Propanedioic acid, phenyl-	180	C9H8O4	002613-89-0	86
3	p-Methylbenzeneboronic acid	136	C7H9BO2	005720-05-8	59
4	Benzeneacetaldehyde	120	C8H8O	000122-78-1	53
5	Thiocyanic acid, phenylmethyl ester	149	C8H7NS	003012-37-1	50





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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

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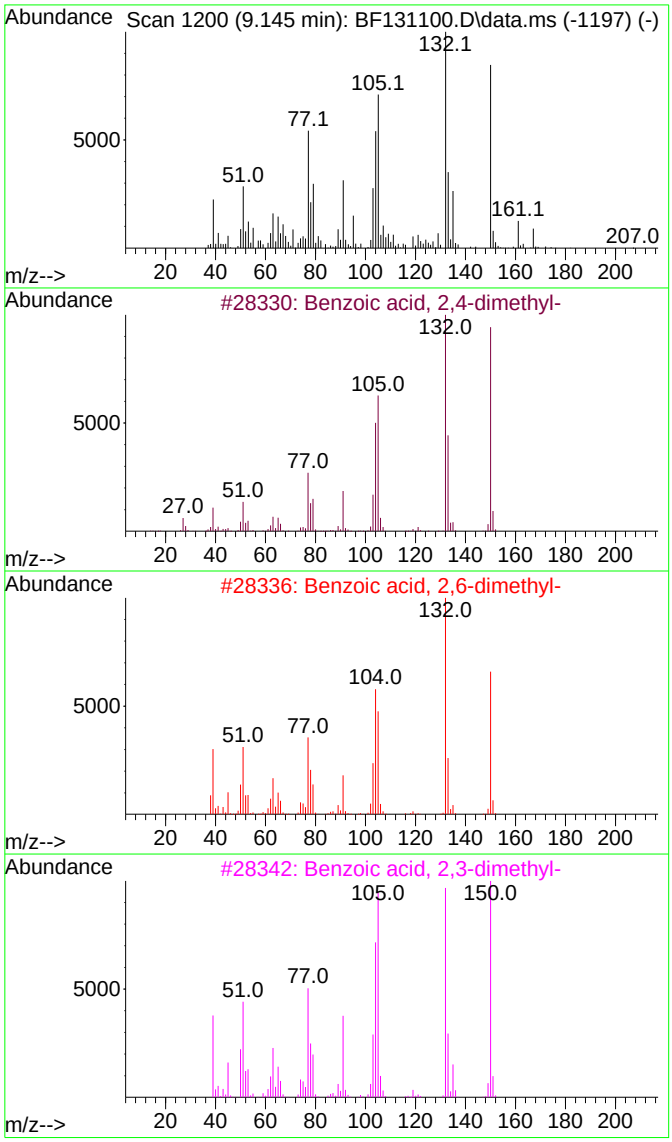
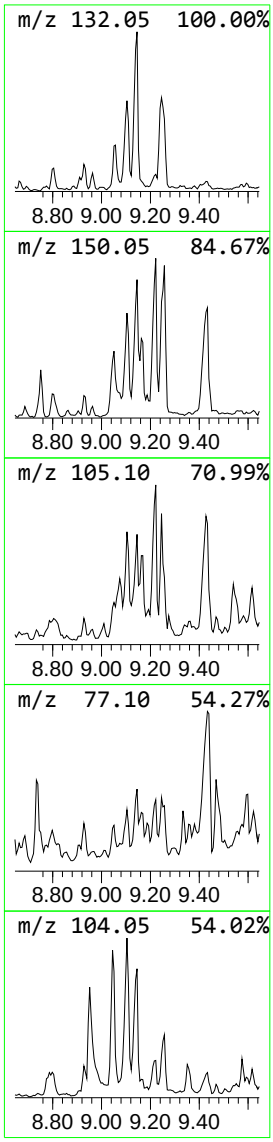
Peak Number 10 Benzoic acid, 2,4-dimethyl- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.145	17.19 ng	520509	Acenaphthene-d10	9.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2,4-dimethyl-	150	C9H10O2	000611-01-8	95
2	Benzoic acid, 2,6-dimethyl-	150	C9H10O2	000632-46-2	90
3	Benzoic acid, 2,3-dimethyl-	150	C9H10O2	000603-79-2	60
4	Benzoic acid, 2,5-dimethyl-	150	C9H10O2	000610-72-0	58
5	Benzamide, 2-(methylamino)-	150	C8H10N2O	007505-81-9	45





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Misc :
ALS Vial : 9 Sample Multiplier: 1

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

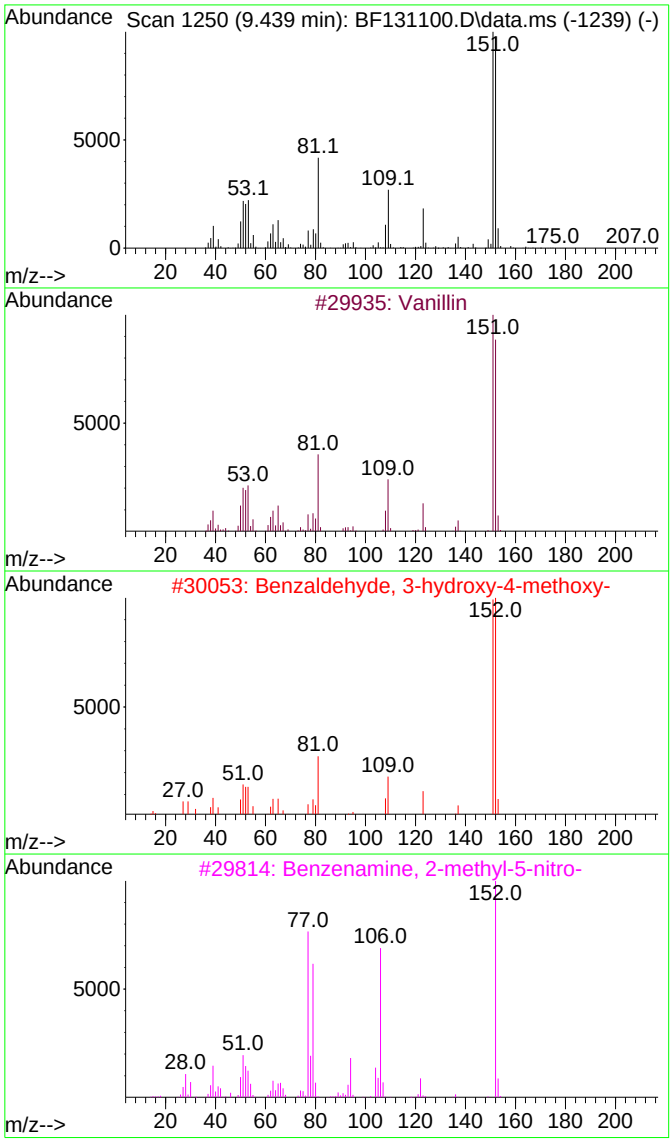
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

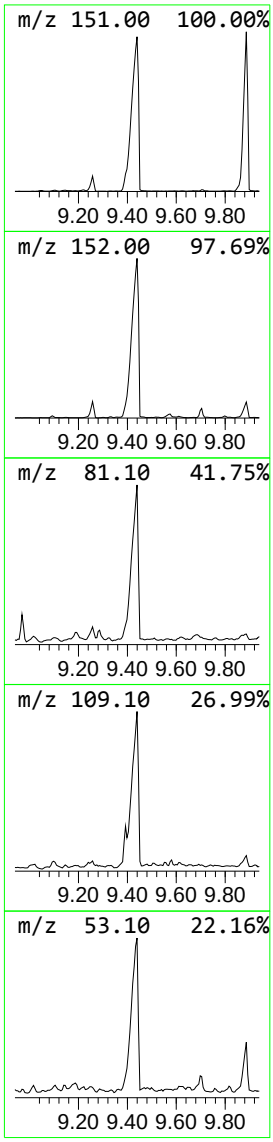
****

Peak Number 11 Vanillin Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.439	245.33 ng	7428780	Acenaphthene-d10	9.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Vanillin	152	C8H8O3	000121-33-5	98
2	Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	97
3	Benzenamine, 2-methyl-5-nitro-	152	C7H8N2O2	000099-55-8	47
4	Benzaldehyde, 2,6-dihydroxy-4-me...	152	C8H8O3	000526-37-4	47
5	Benzaldehyde, 2,4-dihydroxy-6-me...	152	C8H8O3	000487-69-4	43





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Sample : N5340-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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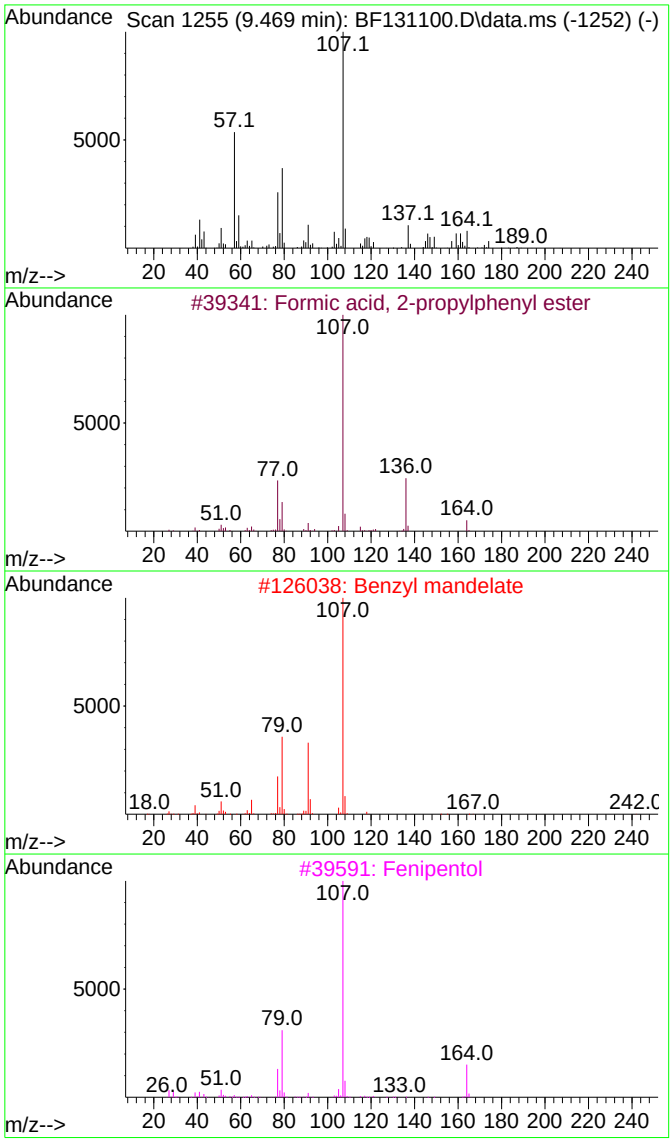
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

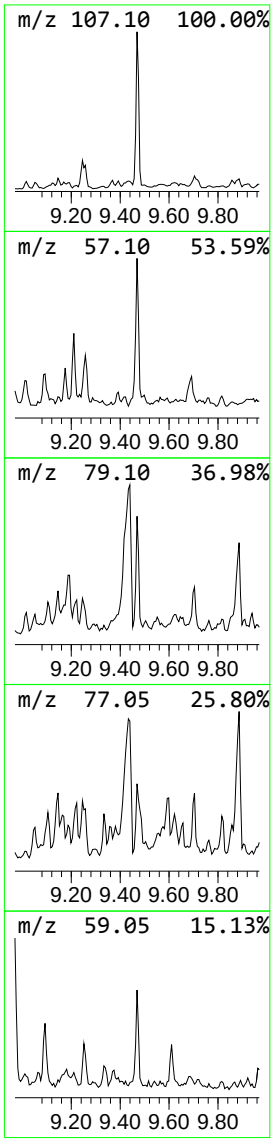
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 Formic acid, 2-propylphenyl... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.469	17.02 ng	515420	Acenaphthene-d10	9.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Formic acid, 2-propylphenyl ester	164	C10H12O2	1010368-96-6	58
2	Benzyl mandelate	242	C15H14O3	000890-98-2	58
3	Fenipentol	164	C11H16O	000583-03-9	58
4	Benzenemethanol, .alpha.-pentyl-	178	C12H18O	004471-05-0	53
5	Mandelamide	151	C8H9NO2	004410-31-5	53





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ALS Vial : 9 Sample Multiplier: 1

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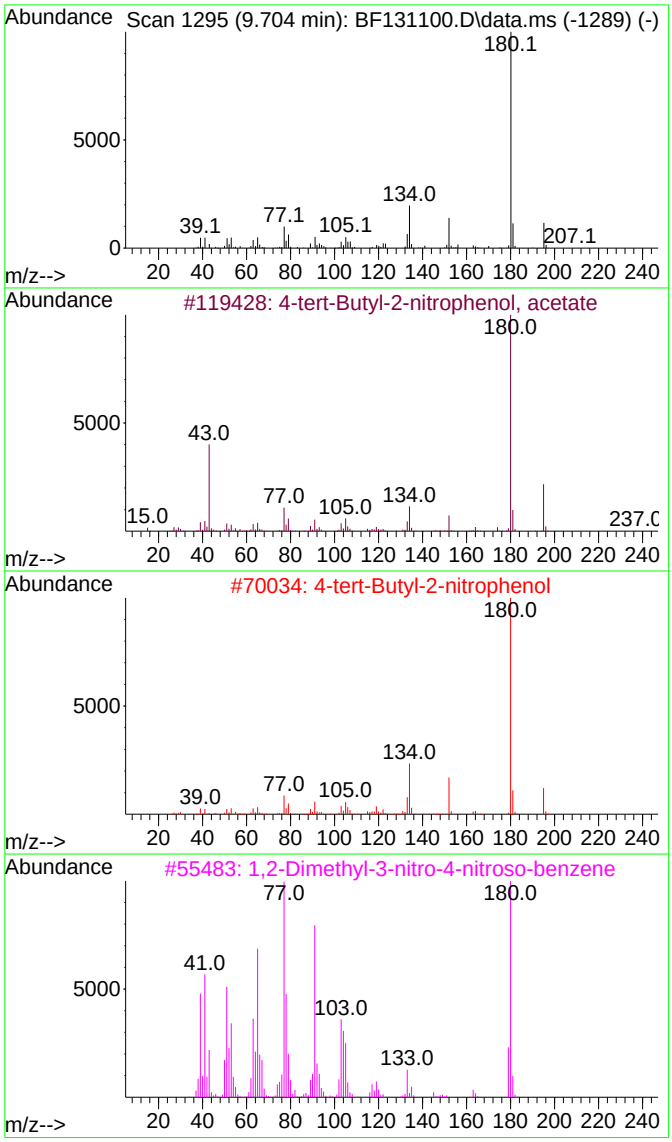
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

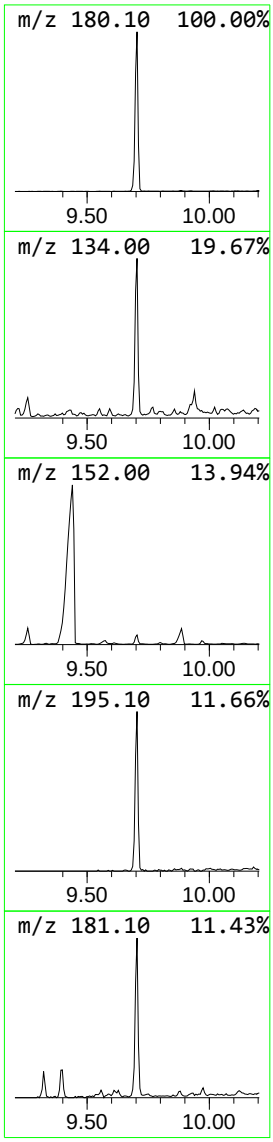
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 4-tert-Butyl-2-nitrophenol,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.704	45.76 ng	1385750	Acenaphthene-d10	9.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-tert-Butyl-2-nitrophenol, acetate	237	C12H15NO4	1000514-77-6	64
2	4-tert-Butyl-2-nitrophenol	195	C10H13NO3	003279-07-0	60
3	1,2-Dimethyl-3-nitro-4-nitroso-b...	180	C8H8N2O3	1000275-00-6	52
4	1,1'-Biphenyl, 4-ethenyl-	180	C14H12	002350-89-2	47
5	5-(4-Nitro-pyrazol-1-yl)-1H-tetr...	181	C4H3N7O2	1000275-34-9	40





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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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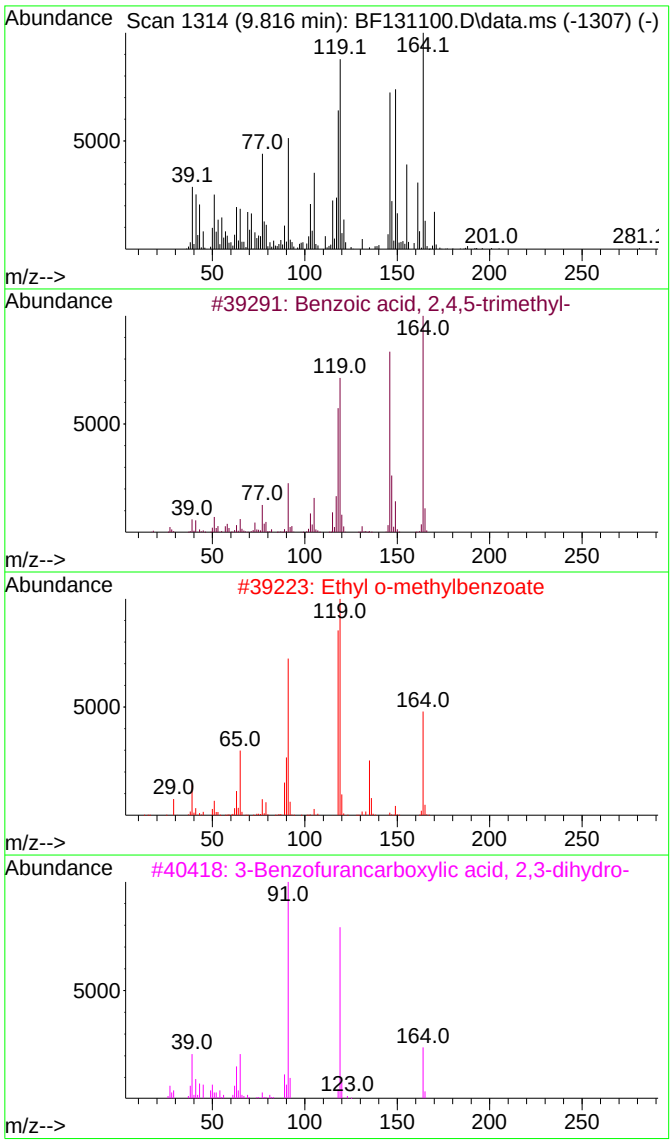
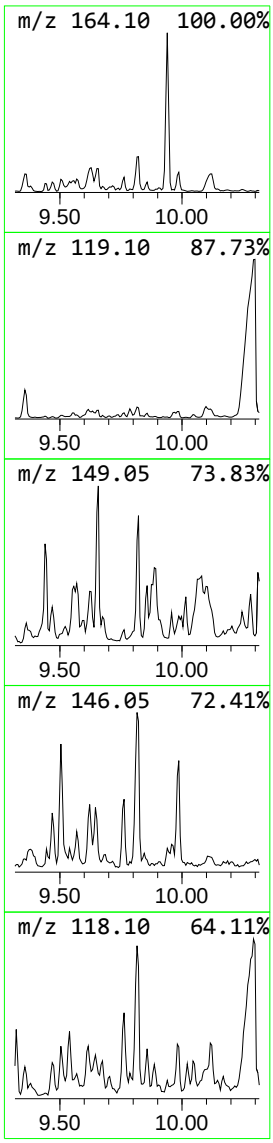
Peak Number 14 Benzoic acid, 2,4,5-trimethyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.816	23.88 ng	723030	Acenaphthene-d10	9.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2,4,5-trimethyl-	164	C10H12O2	000528-90-5	64
2	Ethyl o-methylbenzoate	164	C10H12O2	000087-24-1	41
3	3-Benzofurancarboxylic acid, 2,3...	164	C9H8O3	039891-55-9	38
4	Ethyl m-methylbenzoate	164	C10H12O2	000120-33-2	30
5	1,4-Benzenediamine, N,N,N',N'-te...	164	C10H16N2	000100-22-1	30





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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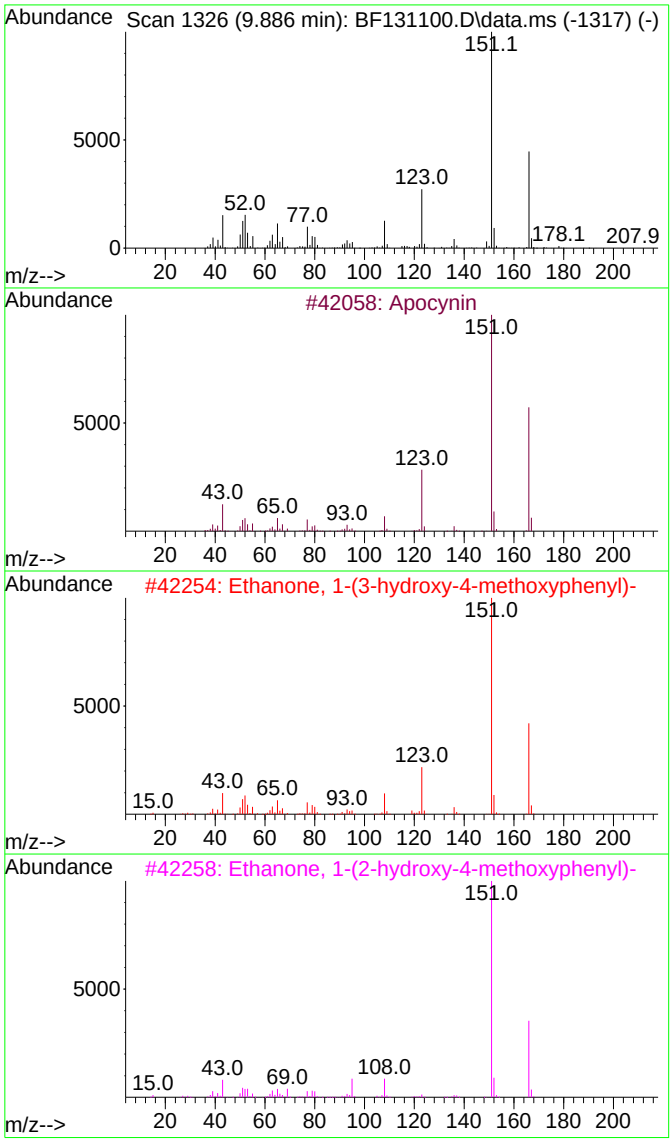
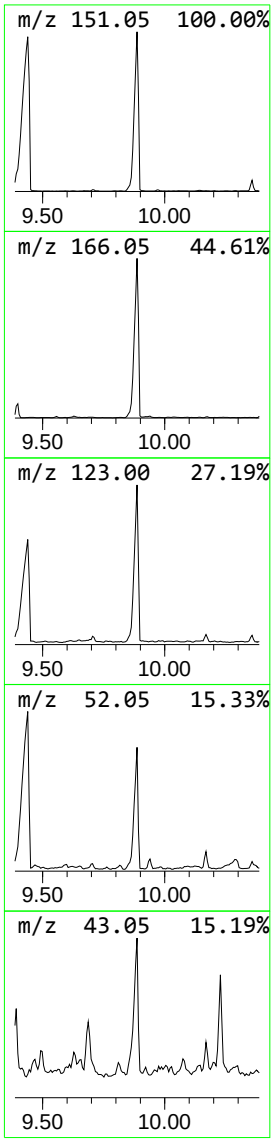
Peak Number 15 Apocynin Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.886	119.33 ng	3613340	Acenaphthene-d10	9.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Apocynin	166	C9H10O3	000498-02-2	95
2	Ethanone, 1-(3-hydroxy-4-methoxy...	166	C9H10O3	006100-74-9	95
3	Ethanone, 1-(2-hydroxy-4-methoxy...	166	C9H10O3	000552-41-0	74
4	Ethanone, 1-[4-(methylthio)phenyl]-	166	C9H10OS	001778-09-2	72
5	2',4'-Dihydroxy-3'-methylacetoph...	166	C9H10O3	010139-84-1	68





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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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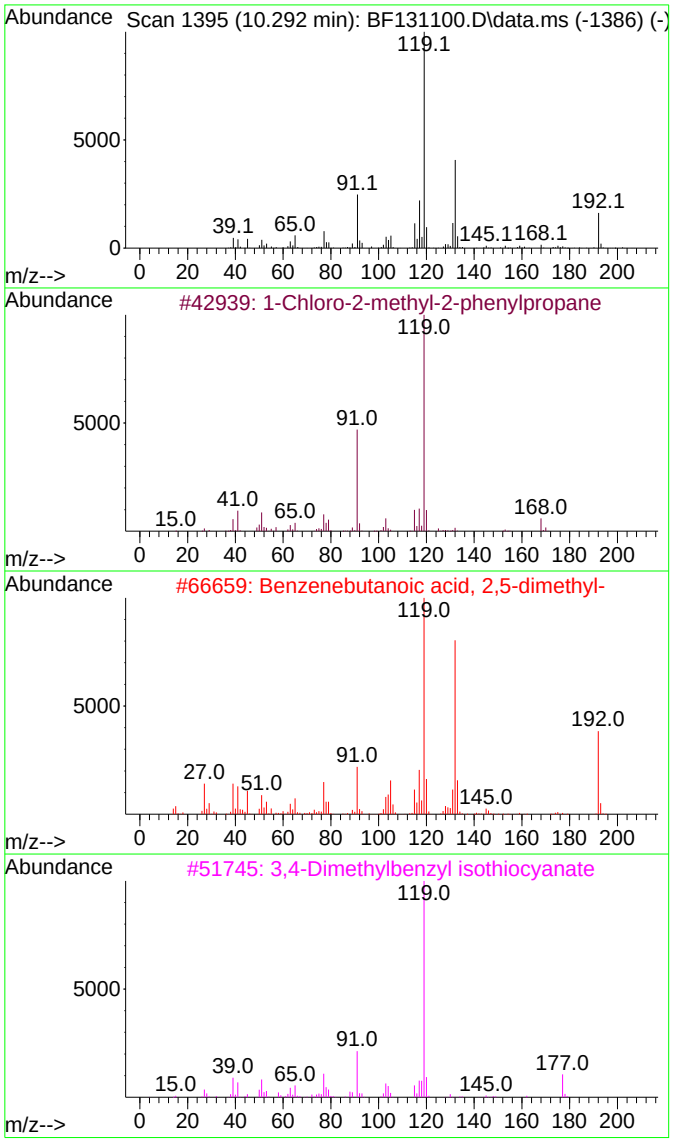
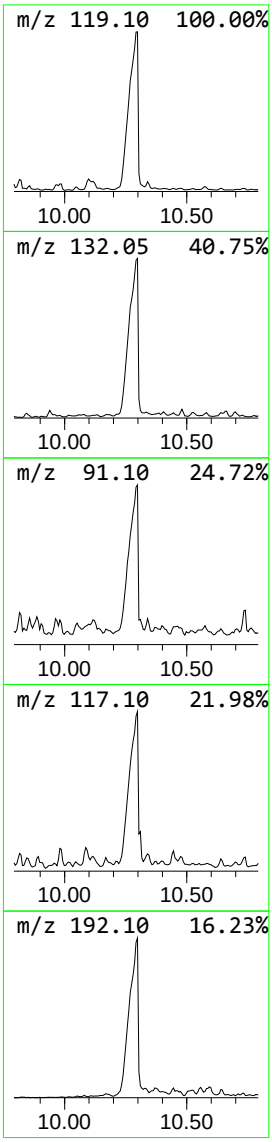
Peak Number 16 unknown10.292 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.292	162.40 ng	4917360	Acenaphthene-d10	9.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Chloro-2-methyl-2-phenylpropane	168	C10H13Cl	000515-40-2	47
2	Benzenebutanoic acid, 2,5-dimethyl-	192	C12H16O2	001453-06-1	45
3	3,4-Dimethylbenzyl isothiocyanate	177	C10H11NS	206559-59-3	43
4	o-Cymene	134	C10H14	000527-84-4	43
5	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110922\
Data File : BF131100.D
Acq On : 09 Nov 2022 22:06
Operator : CG\JU
Sample : N5340-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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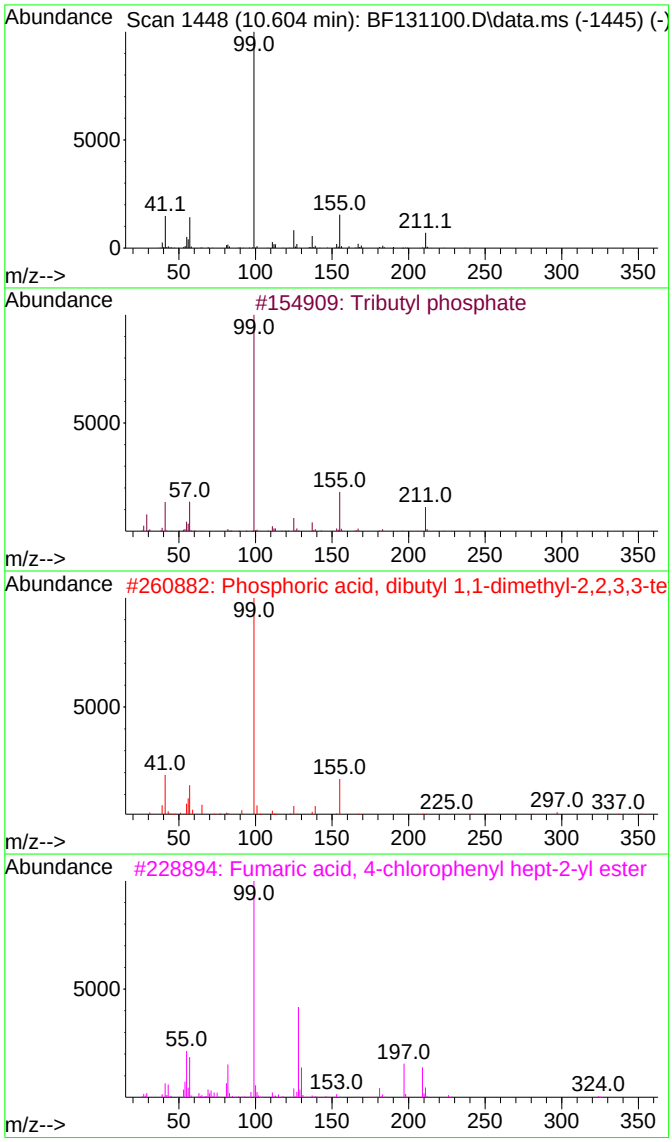
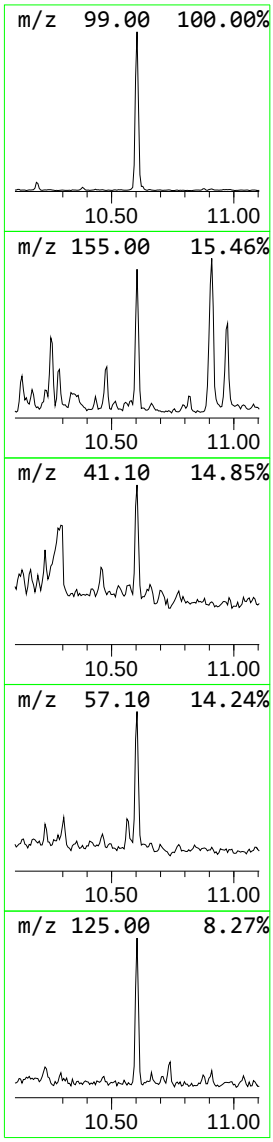
Peak Number 17 Tributyl phosphate Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.604	19.12 ng	579093	Acenaphthene-d10	9.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tributyl phosphate	266	C12H27O4P	000126-73-8	83
2	Phosphoric acid, dibutyl 1,1-dim...	352	C13H25F4O4P	1000298-93-9	72
3	Fumaric acid, 4-chlorophenyl hep...	324	C17H21ClO4	1000405-84-2	50
4	Triisobutyl phosphate	266	C12H27O4P	000126-71-6	50
5	Phosphoric acid, dibutyl 3-trifl...	348	C14H28F3O4P	1000298-93-8	39





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110922\
Data File : BF131100.D
Acq On : 09 Nov 2022 22:06
Operator : CG\JU
Sample : N5340-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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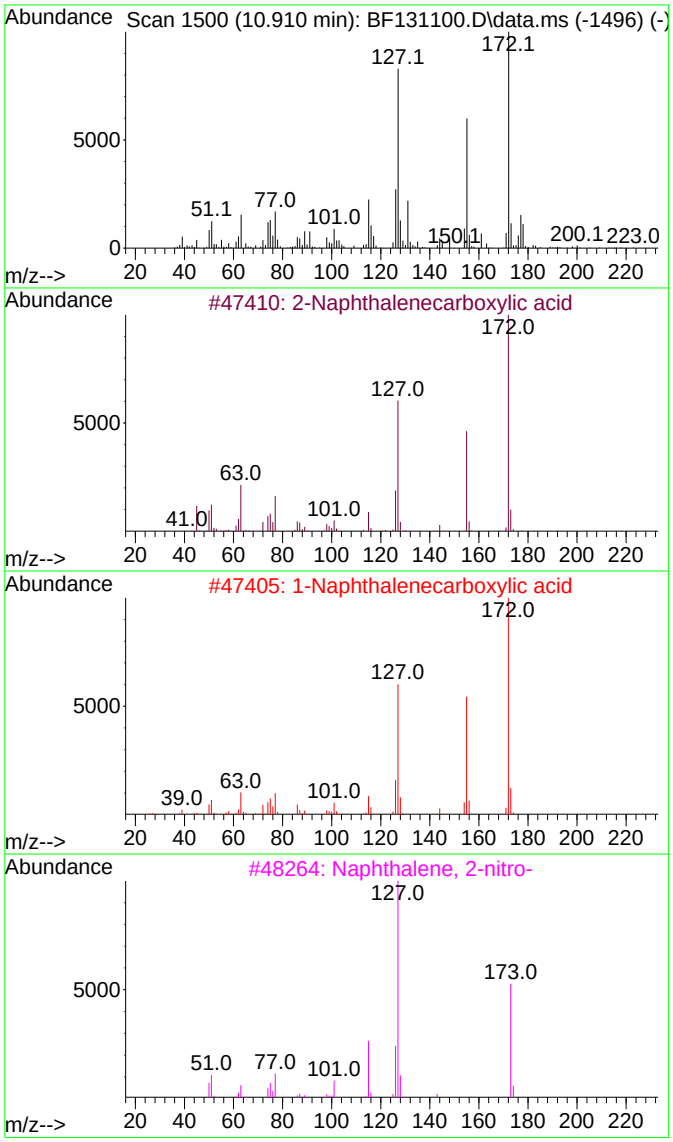
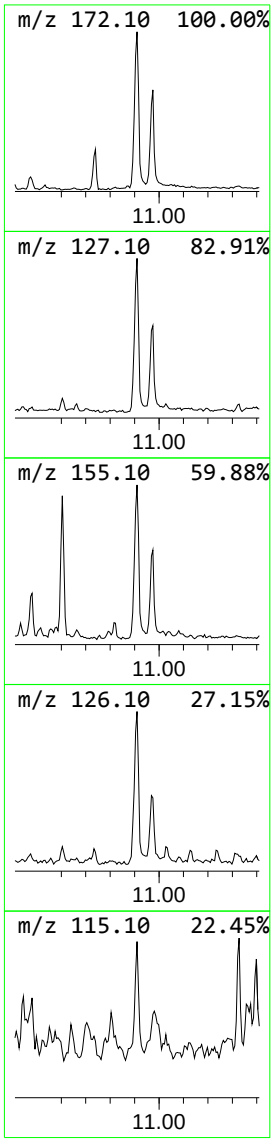
Peak Number 18 2-Naphthalenecarboxylic acid Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.910	18.92 ng	665681	Phenanthrene-d10	11.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Naphthalenecarboxylic acid	172	C11H8O2	000093-09-4	95
2	1-Naphthalenecarboxylic acid	172	C11H8O2	000086-55-5	92
3	Naphthalene, 2-nitro-	173	C10H7NO2	000581-89-5	74
4	2,6-Difluorophenylacetic acid	172	C8H6F2O2	085068-28-6	47
5	1-Naphthamide	171	C11H9NO	002243-81-4	43





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Data File : BF131100.D
Acq On : 09 Nov 2022 22:06
Operator : CG\JU
Sample : N5340-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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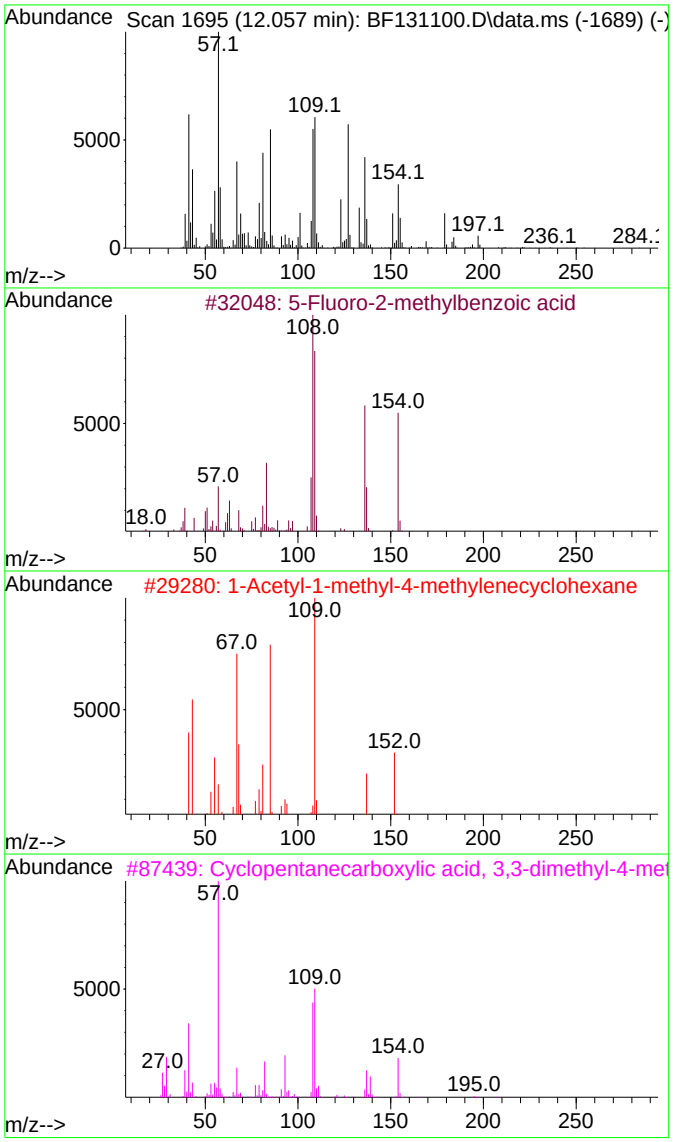
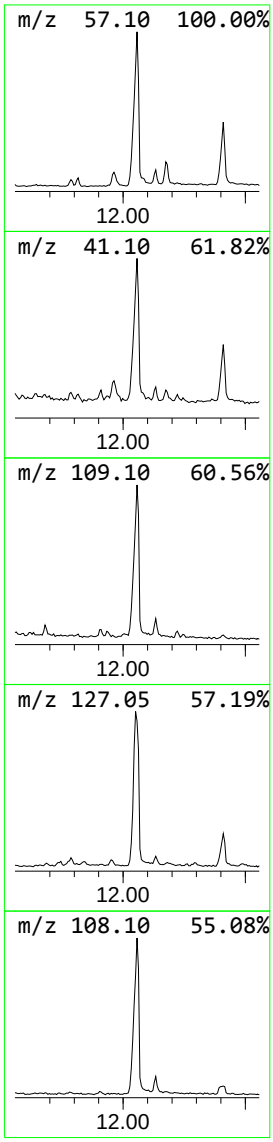
Peak Number 19 unknown12.057 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.057	68.54 ng	2410930	Phenanthrene-d10	11.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-methylbenzoic acid	154	C8H7FO2	033184-16-6	46
2	1-Acetyl-1-methyl-4-methylenecyc...	152	C10H16O	1000424-28-4	30
3	Cyclopentanecarboxylic acid, 3,3...	210	C13H22O2	087753-77-3	22
4	1H-Pyrrole, 4-ethyl-2,3-dimethyl-	123	C8H13N	000491-18-9	22
5	.beta.-Resorcylic acid	154	C7H6O4	000089-86-1	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110922\
Data File : BF131100.D
Acq On : 09 Nov 2022 22:06
Operator : CG\JU
Sample : N5340-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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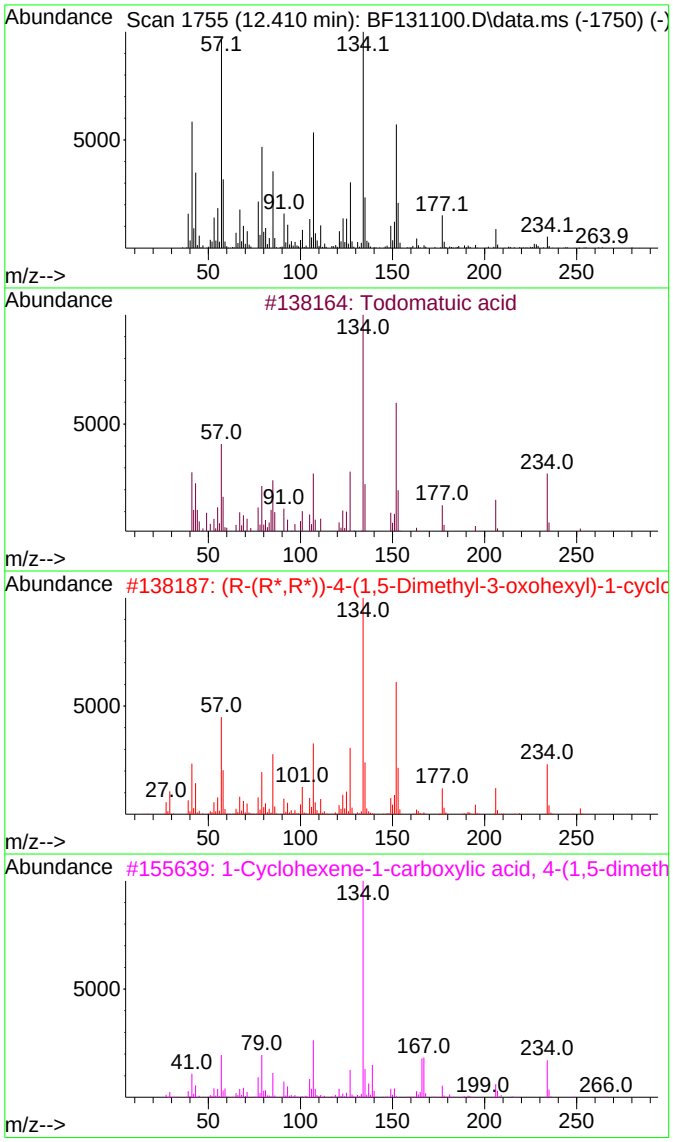
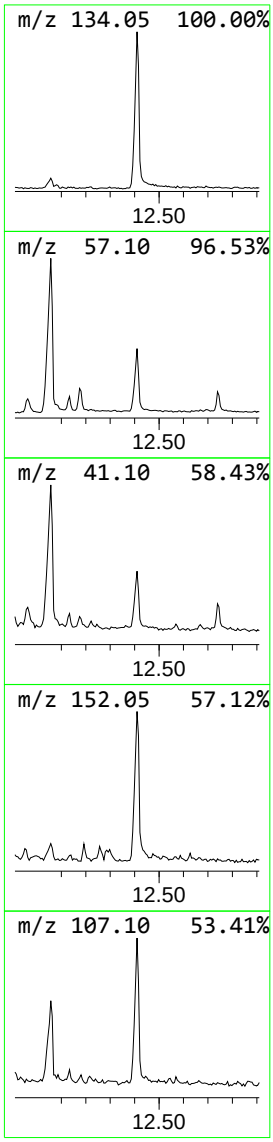
Peak Number 20 Todomatuic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.410	29.69 ng	1044440	Phenanthrene-d10	11.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Todomatuic acid	252	C15H24O3	017844-07-4	80
2	(R-(R*,R*))-4-(1,5-Dimethyl-3-ox...	252	C15H24O3	006753-22-6	72
3	1-Cyclohexene-1-carboxylic acid,...	266	C16H26O3	017904-27-7	58
4	4-Azaindol-2(3H)-one	134	C7H6N2O	032501-05-6	35
5	5H-Pyrrolo(3,2-d)pyrimidin-4-amine	134	C6H6N4	002227-98-7	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110922\
Data File : BF131100.D
Acq On : 09 Nov 2022 22:06
Operator : CG\JU
Sample : N5340-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.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
Butane, 2-metho...	2.193	70.0	ng	2181390	1	6.893	622939	20.0
1,3,5,7-Cyclooc...	5.728	22.4	ng	695988	1	6.893	622939	20.0
unknown6.951	6.951	24.9	ng	774344	1	6.893	622939	20.0
1-Heptene, 3-me...	6.969	33.4	ng	1041390	1	6.893	622939	20.0
unknown7.375	7.375	28.9	ng	901276	1	6.893	622939	20.0
Hexanoic acid, ...	7.898	68.3	ng	5077010	2	8.181	1487110	20.0
Bicyclo[2.2.1]h...	7.928	25.8	ng	1914840	2	8.181	1487110	20.0
endo-Borneol	8.104	24.7	ng	1833780	2	8.181	1487110	20.0
Benzeneacetic acid	8.545	18.6	ng	1380770	2	8.181	1487110	20.0
Benzoic acid, 2...	9.145	17.2	ng	520509	3	9.939	605606	20.0
Vanillin	9.439	245.3	ng	7428780	3	9.939	605606	20.0
Formic acid, 2-...	9.469	17.0	ng	515420	3	9.939	605606	20.0
4-tert-Butyl-2-...	9.704	45.8	ng	1385750	3	9.939	605606	20.0
Benzoic acid, 2...	9.816	23.9	ng	723030	3	9.939	605606	20.0
Apocynin	9.886	119.3	ng	3613340	3	9.939	605606	20.0
unknown10.292	10.292	162.4	ng	4917360	3	9.939	605606	20.0
Tributyl phosphate	10.604	19.1	ng	579093	3	9.939	605606	20.0
2-Naphthaleneca...	10.910	18.9	ng	665681	4	11.433	703534	20.0
unknown12.057	12.057	68.5	ng	2410930	4	11.433	703534	20.0
Todomatuic acid	12.410	29.7	ng	1044440	4	11.433	703534	20.0