LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110522\
Data File : BF131032.D
Acq On : 05 Nov 2022 22:05
Operator : CG\JU
Sample : N5340-07
Misc :
ALS Vial : 19 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-BF102722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131032.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.187	10	17	23	rVB	1393954	1763104	32.24%	2.333%
2	2.316	30	39	45	rVB3	86040	167463	3.06%	0.222%
3	3.422	220	227	234	rBV2	129280	231644	4.24%	0.307%
4	5.122	511	516	520	rBV	368629	374673	6.85%	0.496%
5	5.457	563	573	576	rVB4	90557	223009	4.08%	0.295%
6	5.516	580	583	587	rVV	848708	911789	16.67%	1.207%
7	5.657	599	607	610	rBV	103844	139006	2.54%	0.184%
8	5.699	610	614	616	rVV	174225	187210	3.42%	0.248%
9	5.740	616	621	626	rVV2	556786	668851	12.23%	0.885%
10	6.481	745	747	749	rBV	270223	196933	3.60%	0.261%
11	6.534	752	756	762	rBV2	440278	760777	13.91%	1.007%
12	6.587	762	765	766	rVV	180922	195011	3.57%	0.258%
13	6.610	766	769	771	rVV2	201932	311508	5.70%	0.412%
14	6.634	771	773	774	rVV	243164	241032	4.41%	0.319%
15	6.651	774	776	779	rVB	261119	194400	3.55%	0.257%
16	6.722	785	788	795	rVB	215678	226019	4.13%	0.299%
17	6.904	815	819	822	rBV	586182	560751	10.25%	0.742%
18	6.963	822	829	830	rBV2	615983	765205	13.99%	1.013%
19	6.975	830	831	841	rVV2	737384	1119627	20.47%	1.482%
20	7.057	841	845	855	rVV	1477943	2396733	43.82%	3.172%
21	7.157	859	862	870	rVB3	317658	409127	7.48%	0.541%
22	7.310	877	888	891	rBV2	636186	878681	16.07%	1.163%
23	7.369	891	898	903	rVV5	337929	867117	15.86%	1.148%
24	7.416	903	906	908	rVV2	149293	170474	3.12%	0.226%
25	7.469	908	915	918	rVV2	1783532	2371307	43.36%	3.138%
26	7.504	918	921	926	rVB2	1094015	1101086	20.13%	1.457%
27	7.657	931	947	948	rBV3	457028	1198811	21.92%	1.587%
28	7.745	959	962	965	rBV4	212726	318883	5.83%	0.422%
29	7.804	966	972	974	rBV4	360144	669289	12.24%	0.886%
30	7.940	991	995	998	rVB2	2148284	2128245	38.91%	2.817%
31	7.998	998	1005	1007	rBV2	565117	868795	15.89%	1.150%
32	8.116	1009	1025	1029	rBV4	1542512	5037516	92.11%	6.667%
33	8.187	1035	1037	1039	rVB2	1743016	1337202	24.45%	1.770%
34	8.228	1039	1044	1046	rVB2	3234334	3773637	69.00%	4.994%
35	8.257	1046	1049	1052	rVB5	145005	186583	3.41%	0.247%
36	8.340	1059	1063	1067	rVB5	383194	589296	10.78%	0.780%

LSC Area Percent Report

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Operator : CG\JU
Sample : N5340-07
Misc :
ALS Vial : 19 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-BF102722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	8.392	1067	1072	1074	rVB2	326659	338400	6.19%	0.448%
38	8.422	1074	1077	1080	rBV3	384499	431788	7.90%	0.571%
39	8.469	1083	1085	1092	rVB5	262613	348873	6.38%	0.462%
40	8.545	1092	1098	1099	rBV2	674854	974121	17.81%	1.289%
41	8.616	1104	1110	1114	rBV3	677592	1115281	20.39%	1.476%
42	8.651	1114	1116	1118	rBV	879675	828312	15.15%	1.096%
43	8.745	1126	1132	1133	rBV3	393211	618370	11.31%	0.818%
44	8.763	1133	1135	1139	rVB4	380918	422533	7.73%	0.559%
45	8.804	1139	1142	1147	rVB4	280259	350548	6.41%	0.464%
46	8.892	1154	1157	1160	rBV3	130226	211398	3.87%	0.280%
47	8.934	1161	1164	1169	rVB6	242814	342608	6.26%	0.453%
48	8.975	1169	1171	1174	rVB3	164545	132542	2.42%	0.175%
49	9.016	1174	1178	1181	rBV4	270932	343982	6.29%	0.455%
50	9.104	1188	1193	1196	rVB3	361998	494962	9.05%	0.655%
51	9.139	1196	1199	1201	rBV2	394964	445175	8.14%	0.589%
52	9.175	1201	1205	1209	rVB5	333046	538035	9.84%	0.712%
53	9.210	1209	1211	1214	rVB	367908	362876	6.64%	0.480%
54	9.269	1214	1221	1224	rBV	3161850	3352386	61.30%	4.437%
55	9.310	1224	1228	1231	rVB3	159570	248515	4.54%	0.329%
56	9.345	1231	1234	1236	rBV2	380732	439565	8.04%	0.582%
57	9.445	1241	1251	1254	rVB	3243101	5469000	100.00%	7.238%
58	9.481	1254	1257	1259	rBV	291491	209716	3.83%	0.278%
59	9.592	1274	1276	1278	rBV2	167848	148620	2.72%	0.197%
60	9.681	1288	1291	1293	rBV3	175944	197986	3.62%	0.262%
61	9.716	1294	1297	1300	rVB	726574	646560	11.82%	0.856%
62	9.763	1303	1305	1309	rBV4	164094	158665	2.90%	0.210%
63	9.816	1311	1314	1318	rVB4	438862	502068	9.18%	0.664%
64	9.857	1318	1321	1322	rBV3	255635	219109	4.01%	0.290%
65	9.892	1322	1327	1330	rVV	2198823	2437601	44.57%	3.226%
66	9.951	1334	1337	1339	rVB	654580	482318	8.82%	0.638%
67	9.986	1339	1343	1346	rBV4	353055	308808	5.65%	0.409%
68	10.092	1358	1361	1365	rBV4	325920	381056	6.97%	0.504%
69	10.175	1373	1375	1378	rBV2	227172	213052	3.90%	0.282%
70	10.228	1382	1384	1385	rVV	199412	135771	2.48%	0.180%
71	10.298	1385	1396	1398	rVV	1892948	4443115	81.24%	5.880%
72	10.369	1406	1408	1412	rVB2	164869	143121	2.62%	0.189%
73	10.410	1412	1415	1419	rVB4	171314	233342	4.27%	0.309%
74	10.463	1419	1424	1432	rBV8	225823	545731	9.98%	0.722%
75	10.610	1447	1449	1452	rVB	575649	476764	8.72%	0.631%
76	10.645	1452	1455	1457	rBV4	117861	146641	2.68%	0.194%

LSC Area Percent Report

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Acq On : 05 Nov 2022 22:05
Operator : CG\JU
Sample : N5340-07
Misc :
ALS Vial : 19 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-BF102722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	10.716	1464	1467	1469	rBV2	283431	302361	5.53%	0.400%
78	10.751	1469	1473	1475	rVV	1363671	1363592	24.93%	1.805%
79	10.781	1475	1478	1481	rVB3	328921	304807	5.57%	0.403%
80	10.916	1497	1501	1504	rVB3	467326	459782	8.41%	0.608%
81	11.045	1520	1523	1527	rBV3	258531	287753	5.26%	0.381%
82	11.151	1536	1541	1544	rVB2	251742	305815	5.59%	0.405%
83	11.275	1560	1562	1564	rBV3	157783	132630	2.43%	0.176%
84	11.333	1568	1572	1575	rVB3	255140	335455	6.13%	0.444%
85	11.381	1575	1580	1582	rBV4	160954	267843	4.90%	0.354%
86	11.445	1586	1591	1593	rBV	658716	582093	10.64%	0.770%
87	11.469	1593	1595	1597	rBV	130278	133563	2.44%	0.177%
88	11.963	1675	1679	1690	rVB7	121034	264868	4.84%	0.351%
89	12.069	1691	1697	1705	rBV	1554840	2113410	38.64%	2.797%
90	12.192	1714	1718	1719	rBV2	159806	168780	3.09%	0.223%
91	12.422	1752	1757	1760	rBV2	643237	821854	15.03%	1.088%
92	12.586	1782	1785	1788	rBV	492564	393352	7.19%	0.521%
93	12.751	1810	1813	1817	rBV2	107867	148169	2.71%	0.196%
94	12.927	1840	1843	1846	rBV	185144	153463	2.81%	0.203%
95	13.033	1857	1861	1864	rVB	2302239	2001177	36.59%	2.648%
96	13.410	1922	1925	1930	rBV2	144428	160602	2.94%	0.213%
97	14.092	2038	2041	2044	rVV	452167	379031	6.93%	0.502%
98	14.221	2061	2063	2070	rVB2	97816	125791	2.30%	0.166%
99	14.698	2141	2144	2152	rVB	388056	411178	7.52%	0.544%
100	15.592	2292	2296	2308	rVB	408140	562662	10.29%	0.745%

Sum of corrected areas: 75560139

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110522\
Data File : BF131032.D
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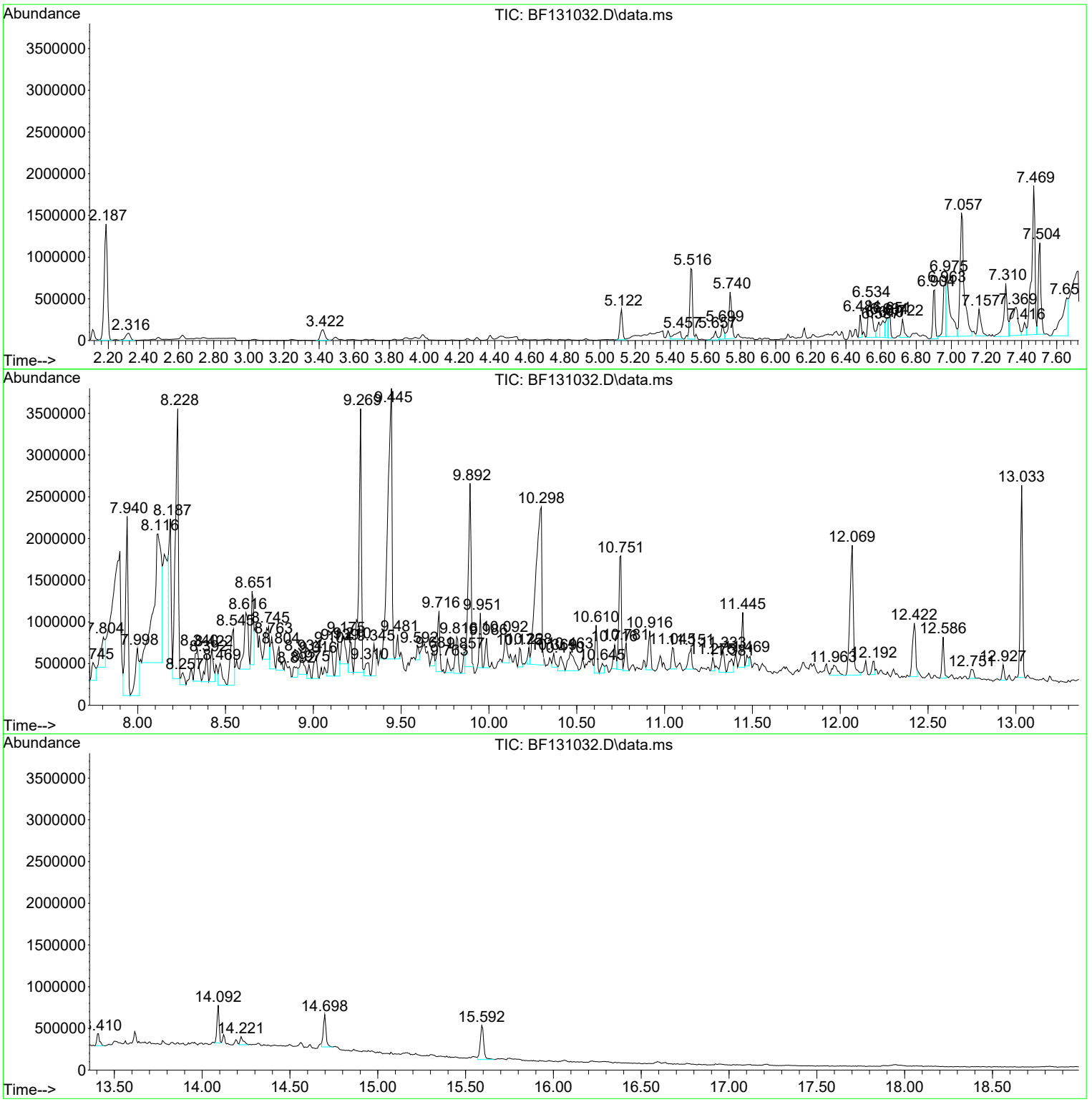
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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\BF110522\
Data File : BF131032.D
Acq On : 05 Nov 2022 22:05
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Sample : N5340-07
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Instrument :
BNA_F
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

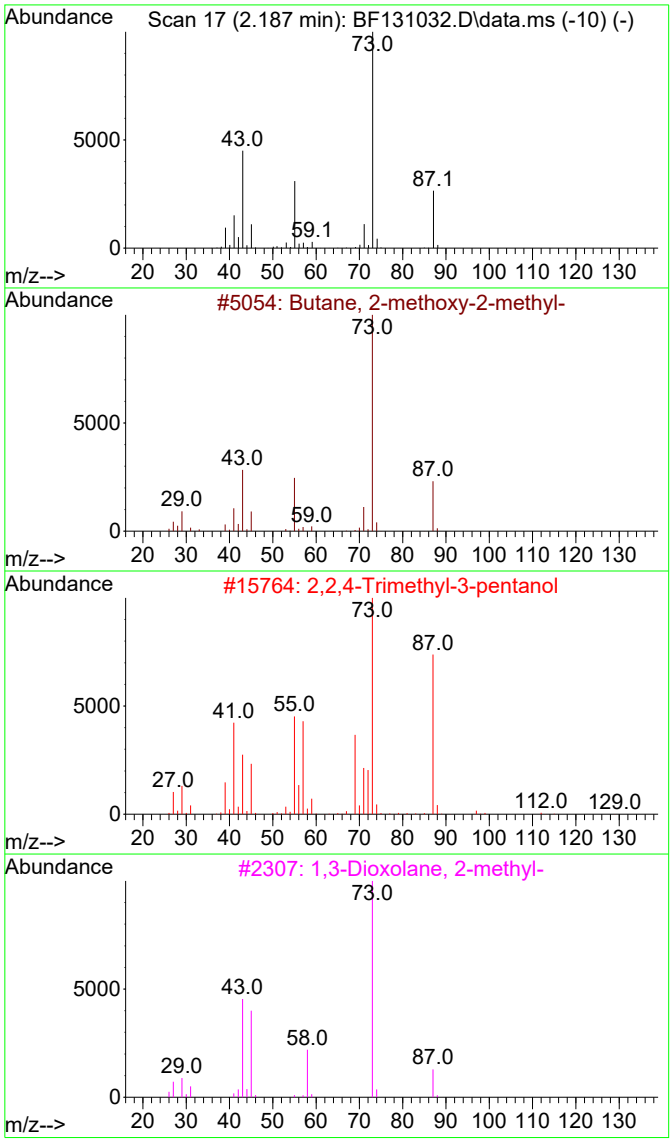
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

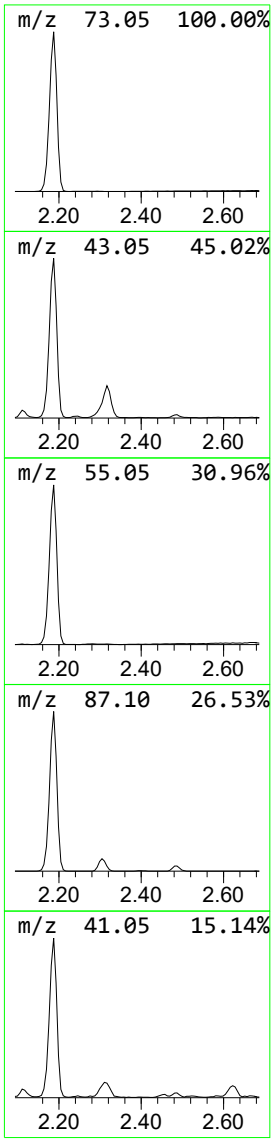
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.187	62.88 ng	1763100	1,4-Dichlorobenzene-d4	6.904

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	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110522\
Data File : BF131032.D
Acq On : 05 Nov 2022 22:05
Operator : CG\JU
Sample : N5340-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

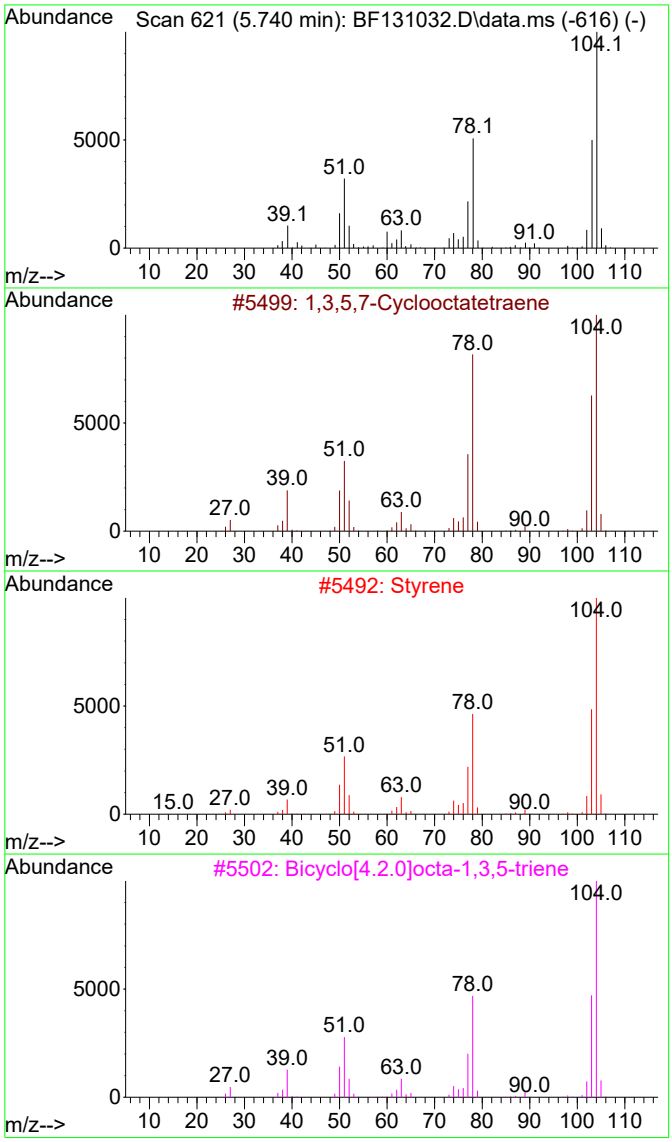
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

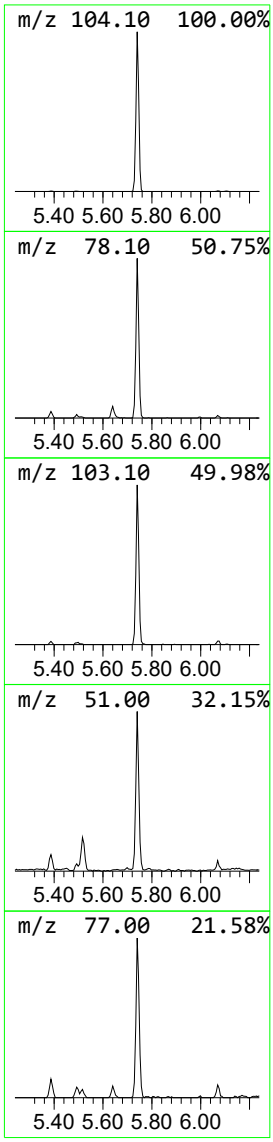
****

Peak Number 2 1,3,5,7-Cyclooctatetraene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.740	23.86 ng	668851	1,4-Dichlorobenzene-d4	6.904

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	2-Pyridinecarbonitrile	104	C6H4N2	000100-70-9	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110522\
Data File : BF131032.D
Acq On : 05 Nov 2022 22:05
Operator : CG\JU
Sample : N5340-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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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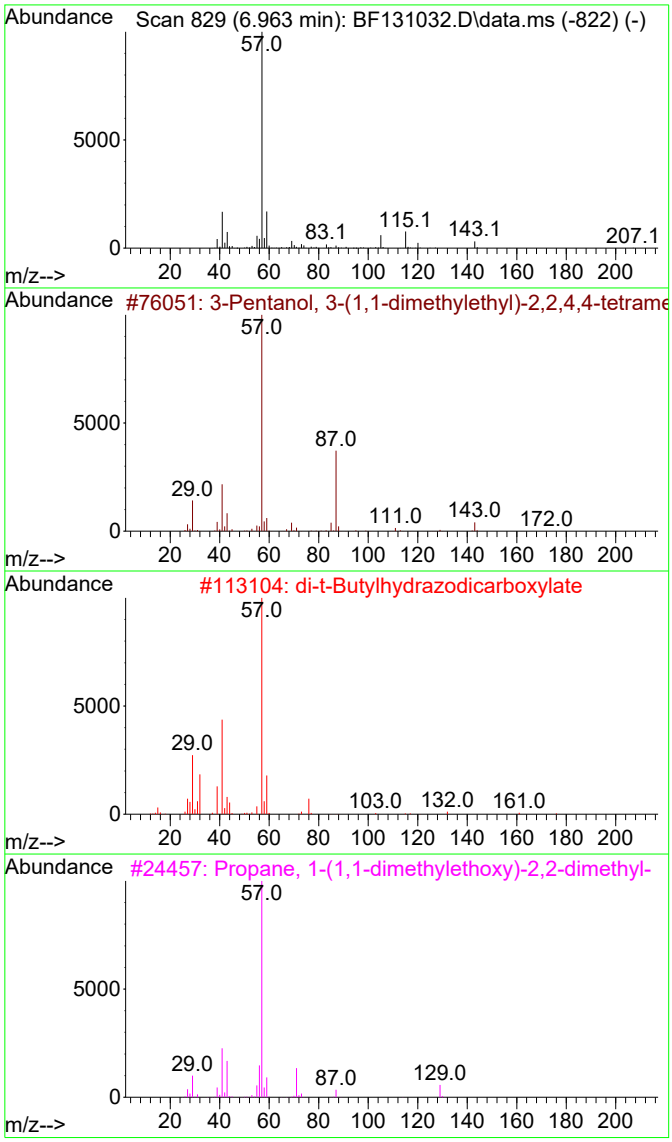
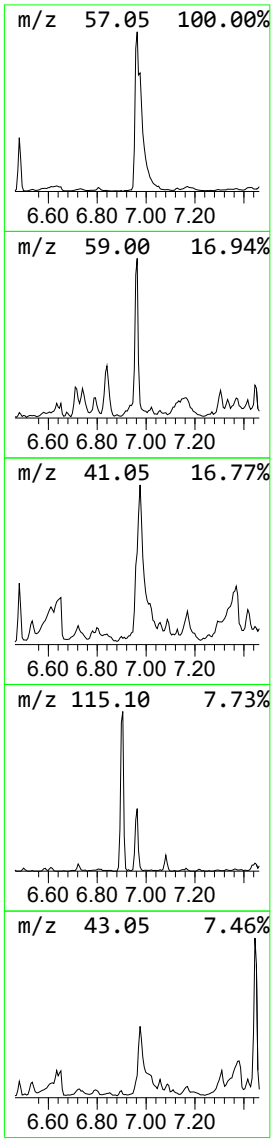
Peak Number 3 unknown6.963 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.963	27.29 ng	765205	1,4-Dichlorobenzene-d4	6.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanol, 3-(1,1-dimethylethyl...	200	C13H28O	041902-42-5	43
2	di-t-Butylhydrazodicarboxylate	232	C10H20N2O4	016466-61-8	33
3	Propane, 1-(1,1-dimethylethoxy)-...	144	C9H20O	032970-46-0	33
4	sec-Butyl isobutyl carbonate	174	C9H18O3	1000372-77-3	28
5	3,5-Octanedione, 2,2,4,7-tetrame...	198	C12H22O2	1000161-72-3	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110522\
Data File : BF131032.D
Acq On : 05 Nov 2022 22:05
Operator : CG\JU
Sample : N5340-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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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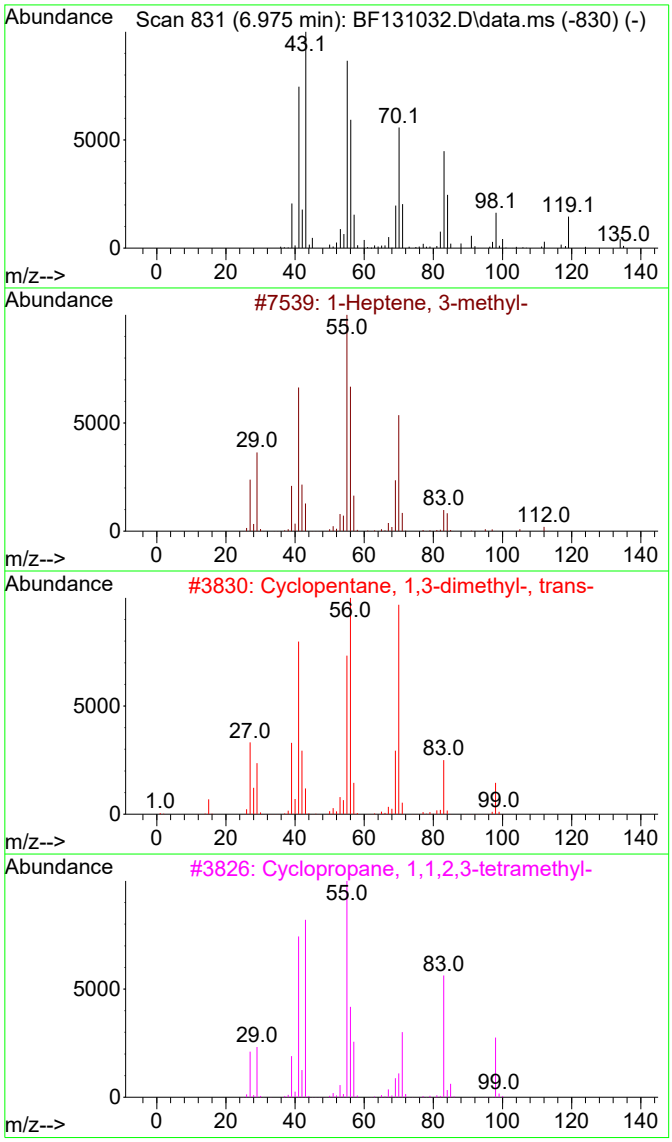
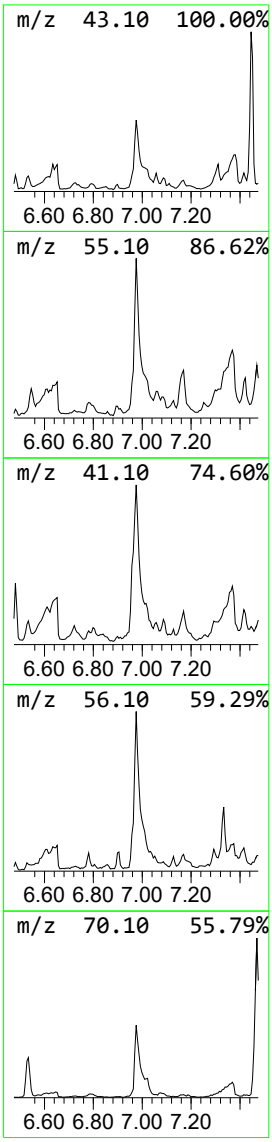
Peak Number 4 1-Heptene, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.975	39.93 ng	1119630	1,4-Dichlorobenzene-d4	6.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptene, 3-methyl-	112	C8H16	004810-09-7	55
2	Cyclopentane, 1,3-dimethyl-, trans-	98	C7H14	001759-58-6	43
3	Cyclopropane, 1,1,2,3-tetramethyl-	98	C7H14	074752-93-5	43
4	Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	43
5	1-Pentanol, 3,4-dimethyl-	116	C7H16O	006570-87-2	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110522\
Data File : BF131032.D
Acq On : 05 Nov 2022 22:05
Operator : CG\JU
Sample : N5340-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

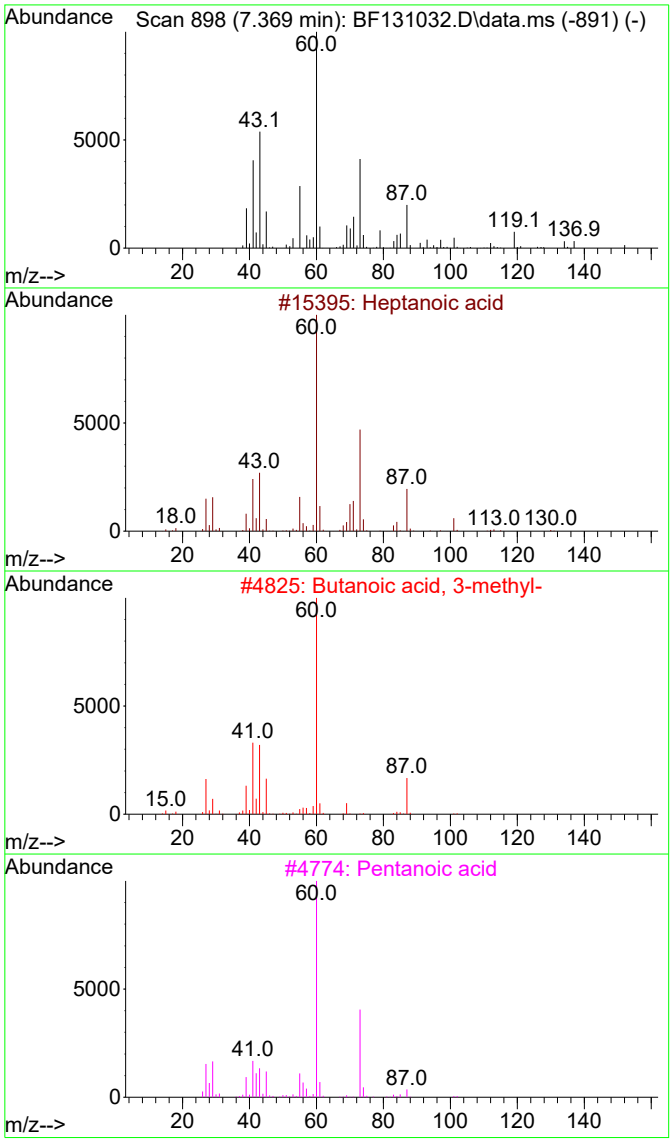
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

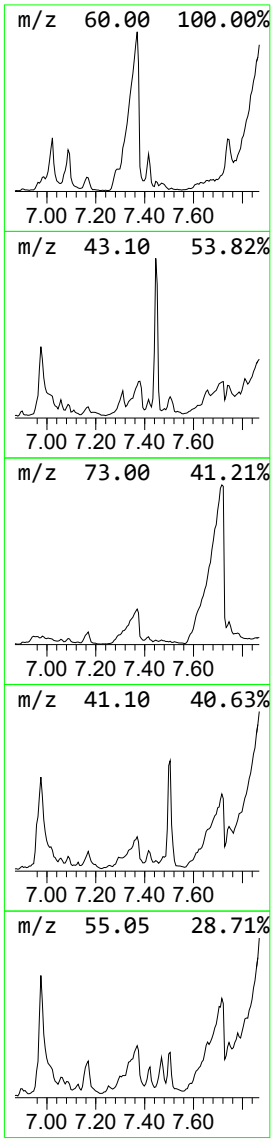
****

Peak Number 5 Heptanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.369	30.93 ng	867117	1,4-Dichlorobenzene-d4	6.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanoic acid	130	C7H14O2	000111-14-8	78
2	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	58
3	Pentanoic acid	102	C5H10O2	000109-52-4	58
4	Ethyl .alpha.-d-glucopyranoside	208	C8H16O6	019467-01-7	56
5	Acetamide, N-(.beta.-mercaptoeth...	119	C4H9NOS	001190-73-4	50





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Acq On : 05 Nov 2022 22:05
Operator : CG\JU
Sample : N5340-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

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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

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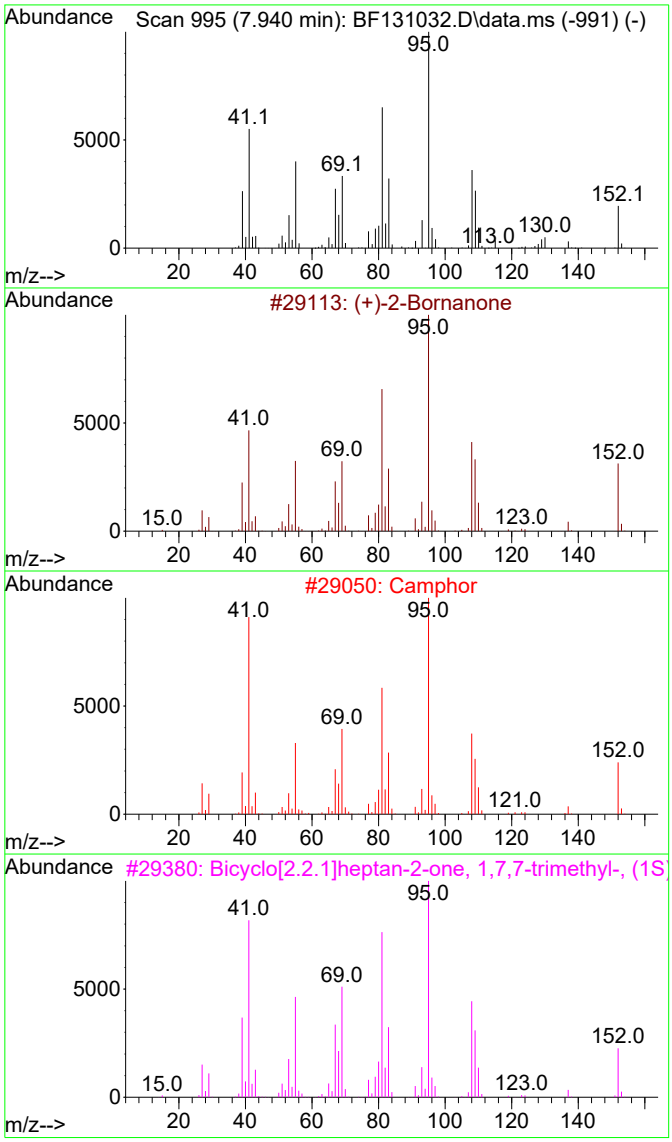
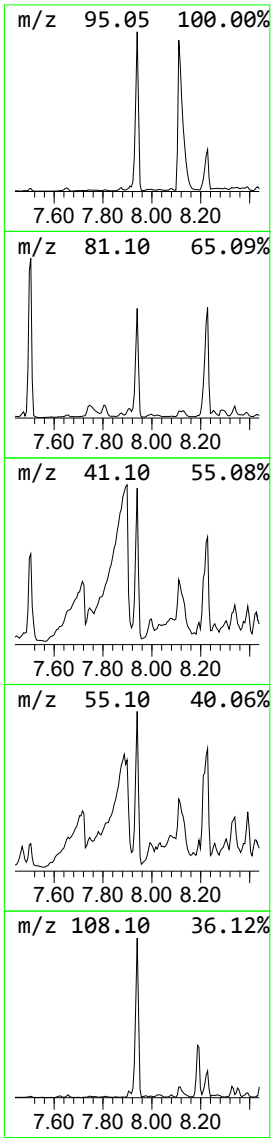
Peak Number 6 (+)-2-Bornanone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.940	31.83 ng	2128250	Naphthalene-d8	8.187

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-2-Bornanone	152	C10H16O	000464-49-3	97
2	Camphor	152	C10H16O	000076-22-2	96
3	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	95
4	5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	006752-80-3	58
5	2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	47





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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

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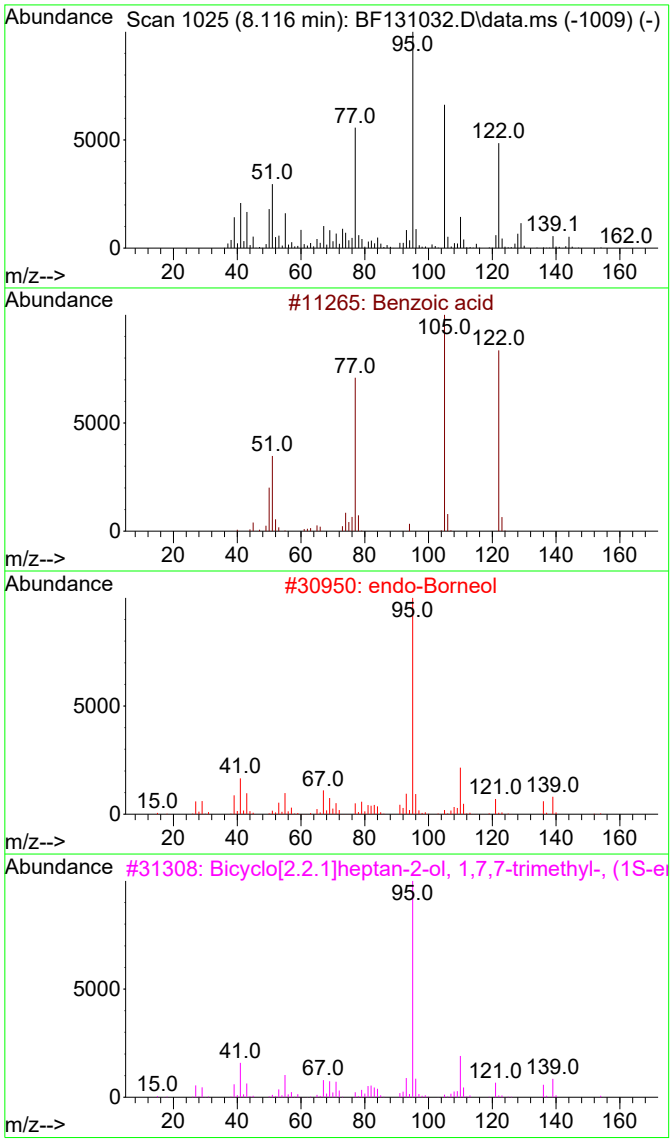
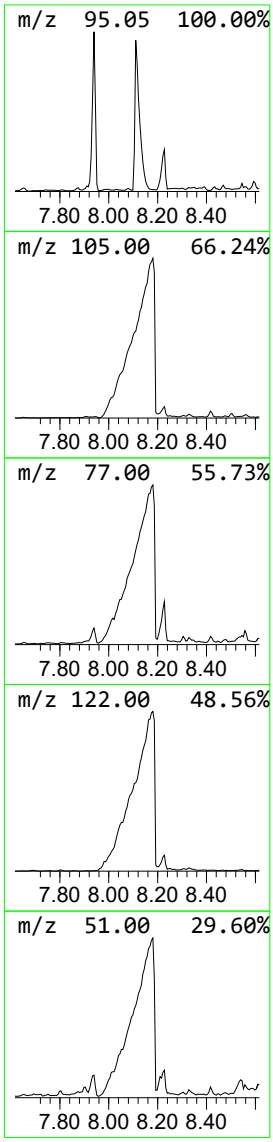
Peak Number 7 endo-Borneol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.116	75.34 ng	5037520	Naphthalene-d8	8.187

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid	122	C7H6O2	000065-85-0	87
2	endo-Borneol	154	C10H18O	000507-70-0	80
3	Bicyclo[2.2.1]heptan-2-ol, 1,7,7...	154	C10H18O	000464-45-9	38
4	Benzoic acid, silver(1+) salt	228	C7H5AgO2	000532-31-0	38
5	Cyclobutane-1,1-dicarboxamide, N...	382	C20H18N2O6	1000253-25-3	38





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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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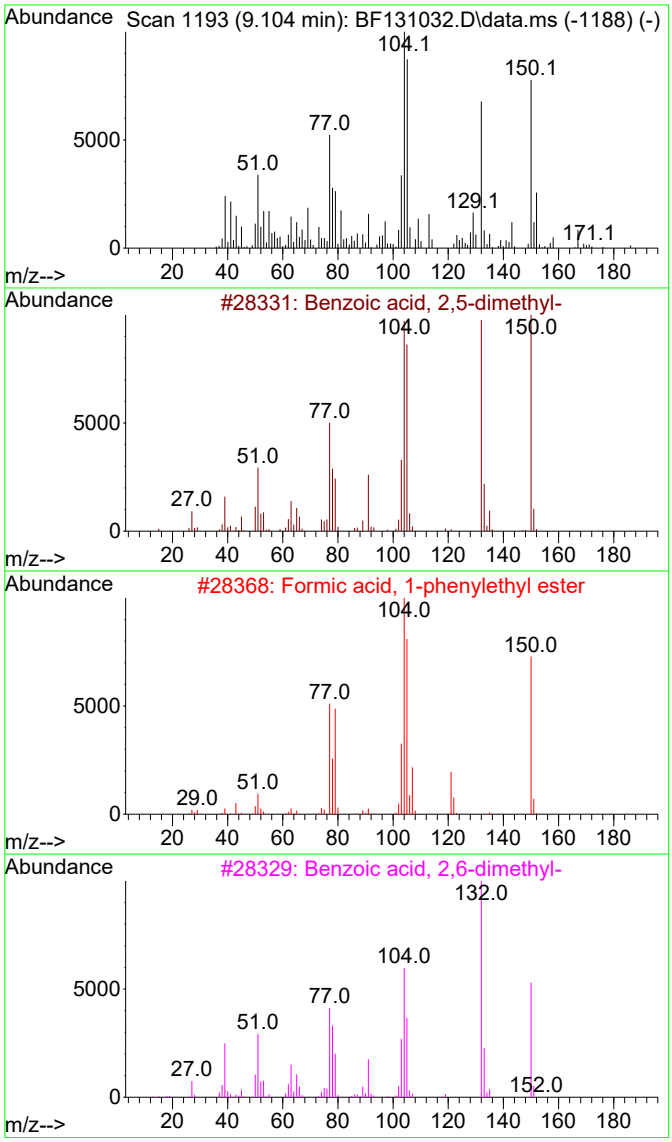
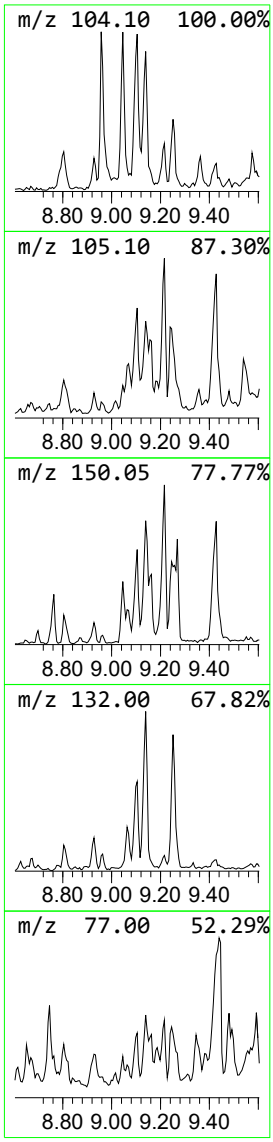
Peak Number 8 Benzoic acid, 2,5-dimethyl- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.104	20.52 ng	494962	Acenaphthene-d10	9.951

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2,5-dimethyl-	150	C9H10O2	000610-72-0	93
2	Formic acid, 1-phenylethyl ester	150	C9H10O2	1000368-94-1	70
3	Benzoic acid, 2,6-dimethyl-	150	C9H10O2	000632-46-2	70
4	para-Methylbenzyl formate	150	C9H10O2	1000368-93-7	64
5	Benzoic acid, 2,3-dimethyl-	150	C9H10O2	000603-79-2	62





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Sample : N5340-07
Misc :
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Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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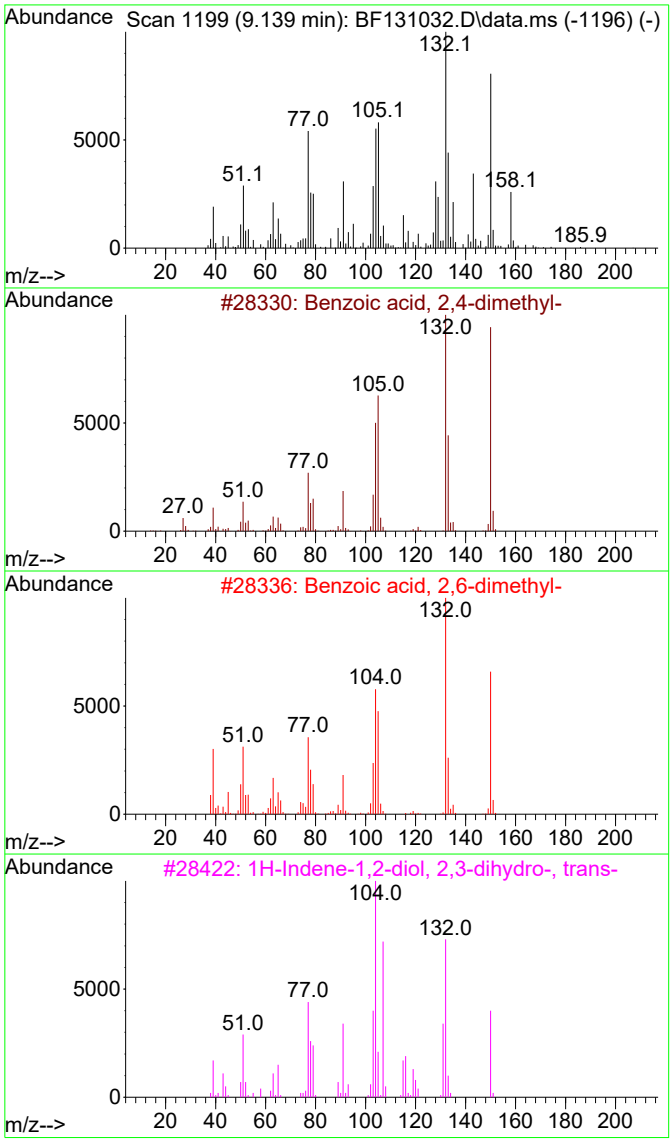
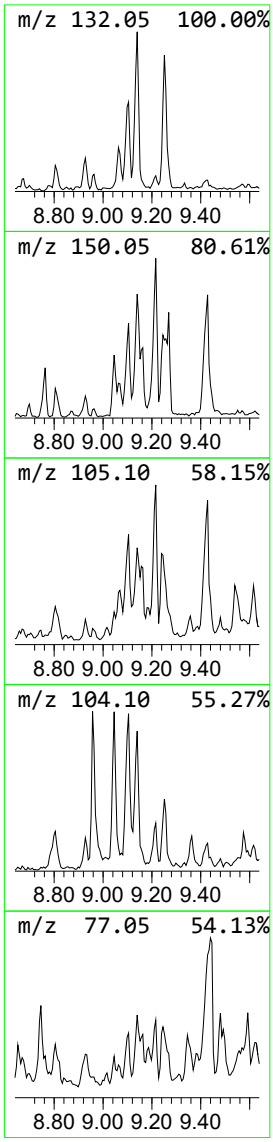
Peak Number 9 Benzoic acid, 2,4-dimethyl- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.139	18.46 ng	445175	Acenaphthene-d10	9.951

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	91
3	1H-Indene-1,2-diol, 2,3-dihydro-...	150	C9H10O2	004647-43-2	49
4	Benzoic acid, 2,3-dimethyl-	150	C9H10O2	000603-79-2	46
5	Isoquinoline, 1,2,3,4-tetrahydro-	133	C9H11N	000091-21-4	46





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ALS Vial : 19 Sample Multiplier: 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

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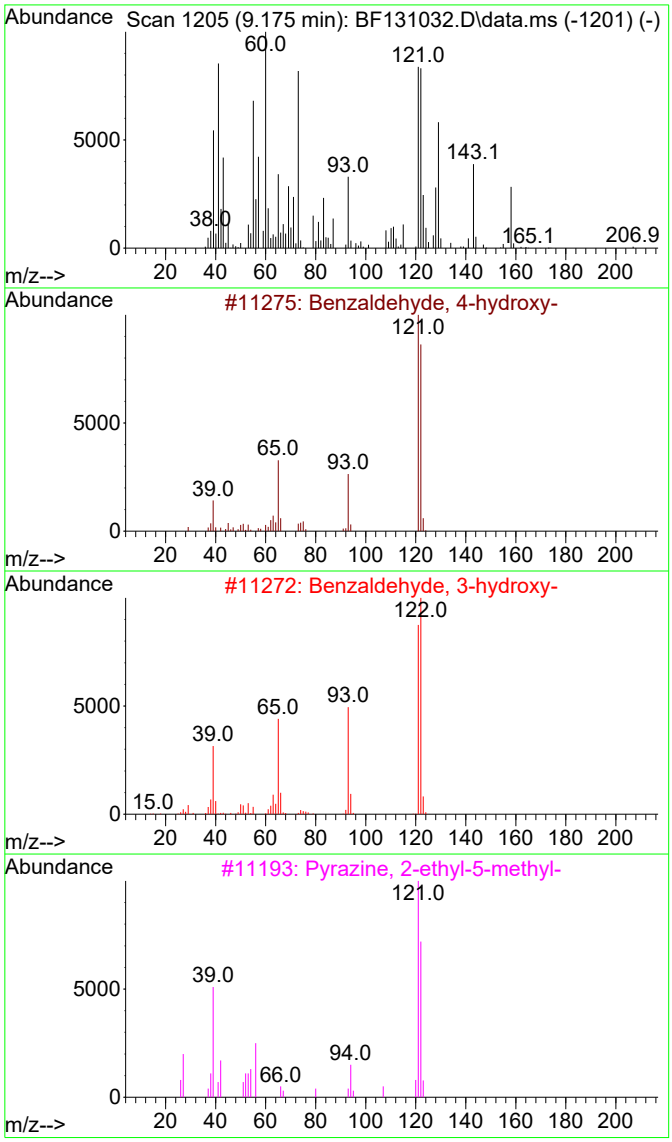
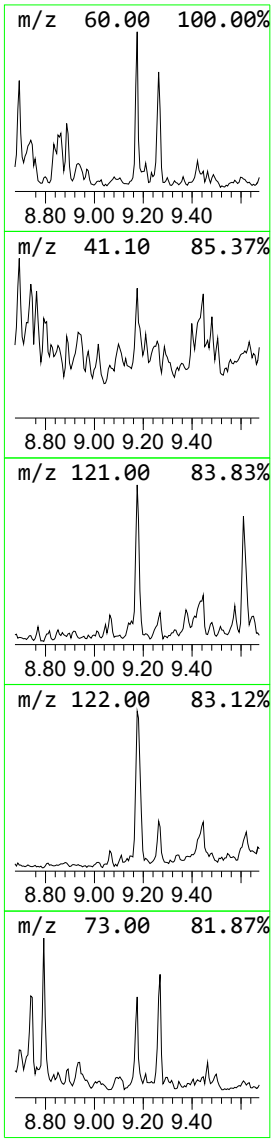
Peak Number 10 Benzaldehyde, 4-hydroxy- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.175	22.31 ng	538035	Acenaphthene-d10	9.951

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 4-hydroxy-	122	C7H6O2	000123-08-0	80
2	Benzaldehyde, 3-hydroxy-	122	C7H6O2	000100-83-4	42
3	Pyrazine, 2-ethyl-5-methyl-	122	C7H10N2	013360-64-0	38
4	Benzaldehyde, 2-hydroxy-	122	C7H6O2	000090-02-8	30
5	1,3-Benzenediamine, 4-methyl-	122	C7H10N2	000095-80-7	30





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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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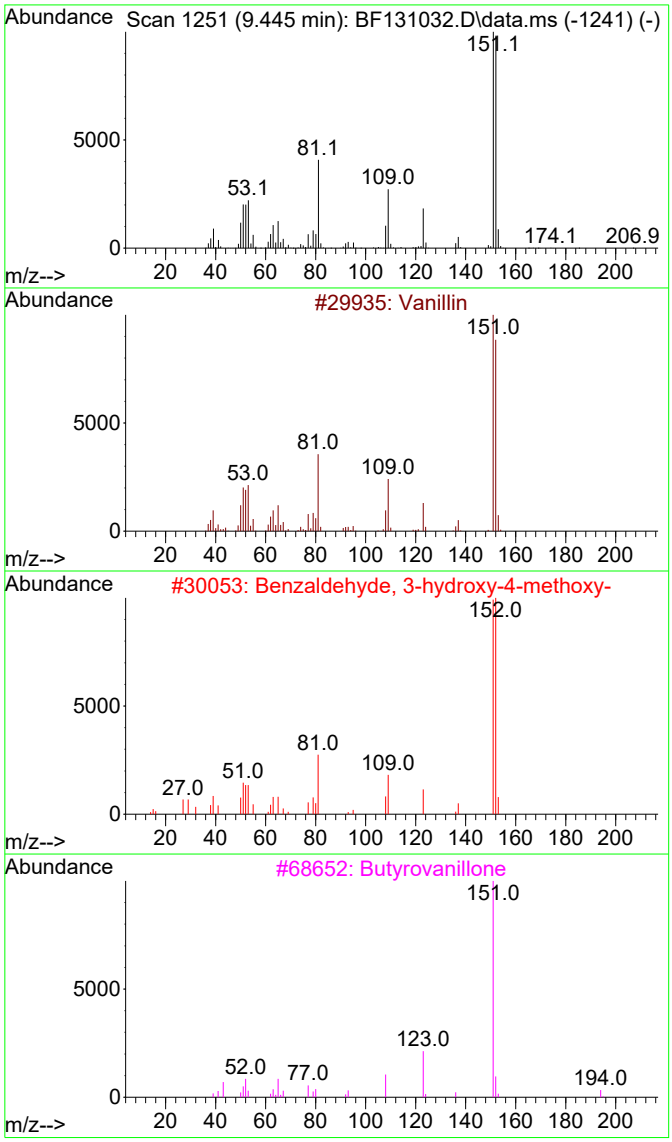
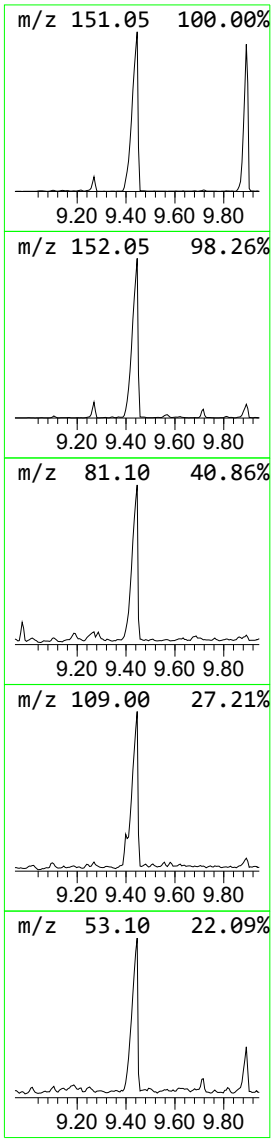
Peak Number 11 Vanillin Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.445	226.78 ng	5469000	Acenaphthene-d10	9.951

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	Butyrovanillone	194	C11H14O3	064142-23-0	43
4	Benzaldehyde, 2-hydroxy-4-methoxy-	152	C8H8O3	000673-22-3	43
5	Benzaldehyde, 2,4-dihydroxy-6-me...	152	C8H8O3	000487-69-4	38





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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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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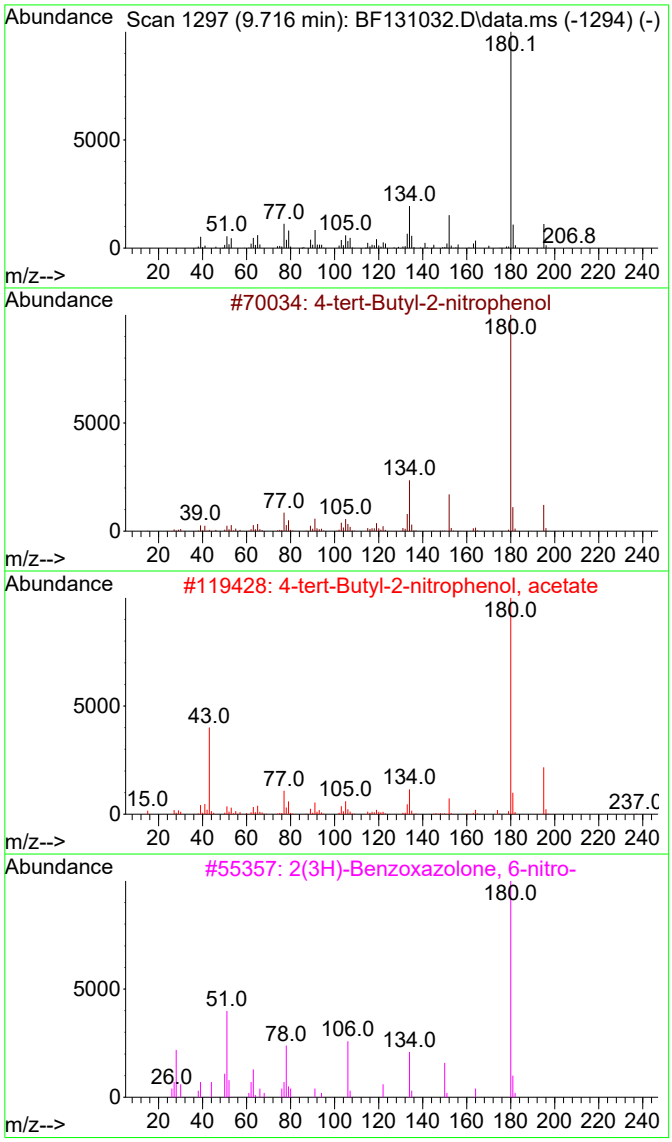
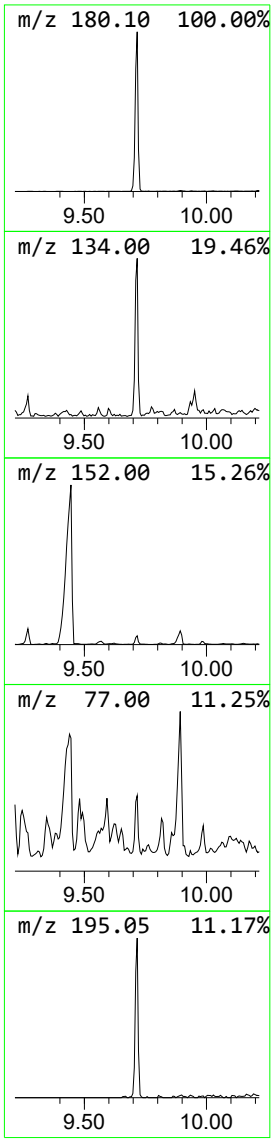
Peak Number 12 4-tert-Butyl-2-nitrophenol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.716	26.81 ng	646560	Acenaphthene-d10	9.951

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-tert-Butyl-2-nitrophenol	195	C10H13NO3	003279-07-0	94
2	4-tert-Butyl-2-nitrophenol, acetate	237	C12H15NO4	1000514-77-6	83
3	2(3H)-Benzoxazolone, 6-nitro-	180	C7H4N2O4	004694-91-1	53
4	4,7-Phenanthroline	180	C12H8N2	000230-07-9	50
5	Propenoic acid, 3-(1-ethyl-5-met...	180	C9H12N2O2	1000272-91-9	50





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ALS Vial : 19 Sample Multiplier: 1

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

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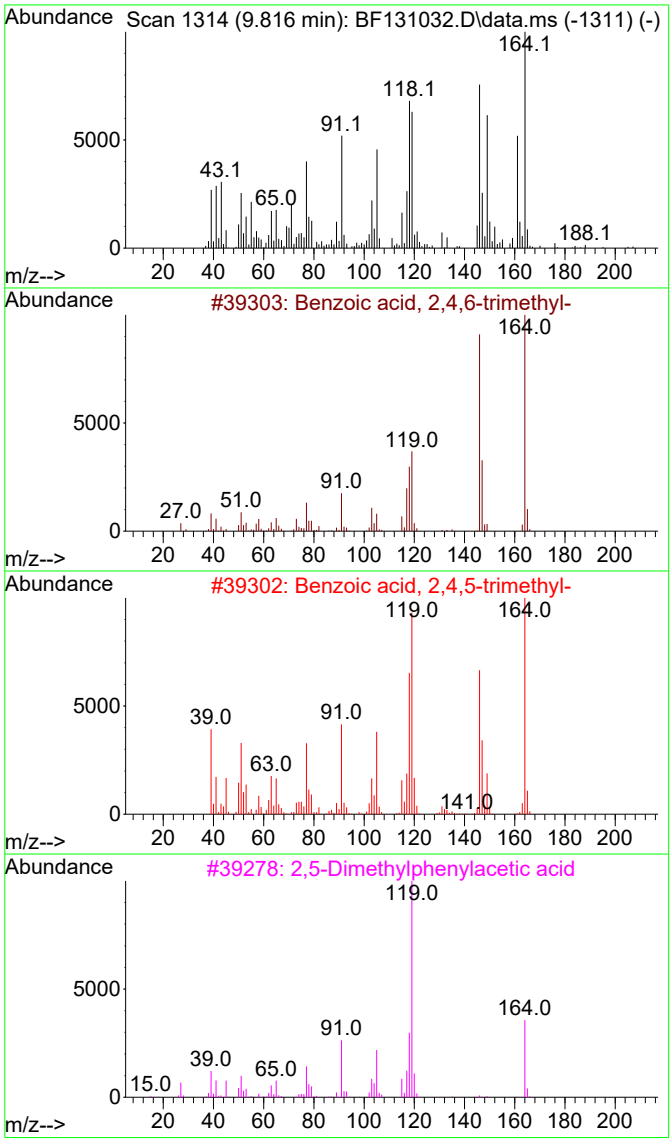
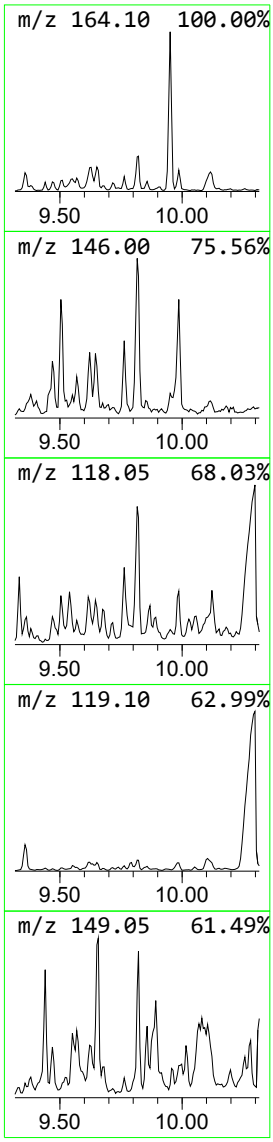
Peak Number 13 Benzoic acid, 2,4,6-trimethyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.816	20.82 ng	502068	Acenaphthene-d10	9.951

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2,4,6-trimethyl-	164	C10H12O2	000480-63-7	89
2	Benzoic acid, 2,4,5-trimethyl-	164	C10H12O2	000528-90-5	64
3	2,5-Dimethylphenylacetic acid	164	C10H12O2	1000342-65-5	46
4	1H-Indole, 5-methoxy-2-methyl-	161	C10H11NO	001076-74-0	35
5	5-Hydroxyindole, N-methyl-, meth...	161	C10H11NO	1000333-38-4	25





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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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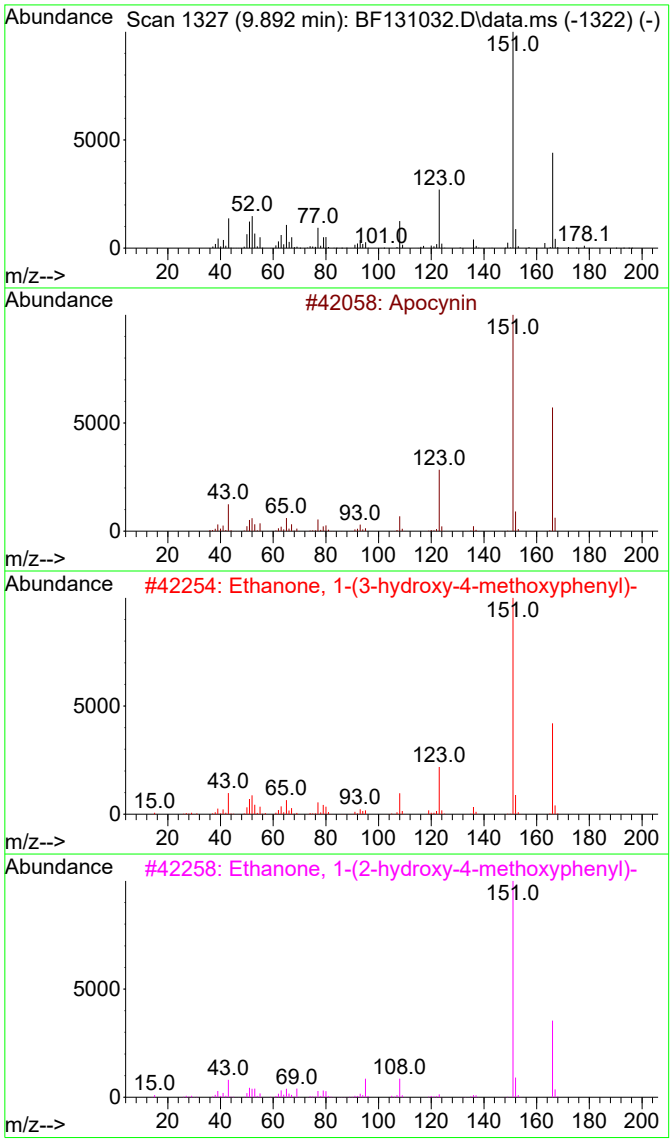
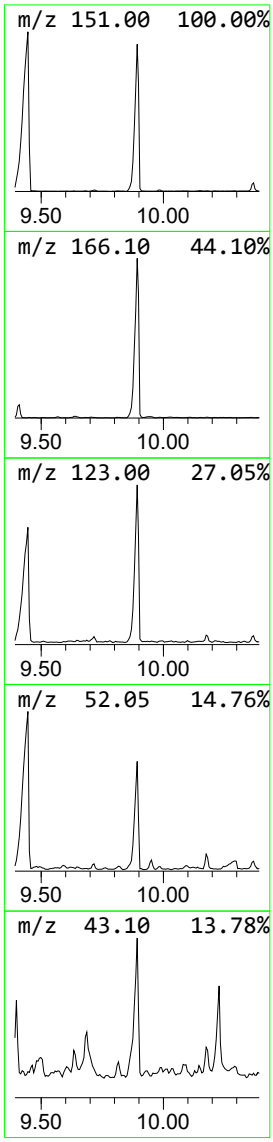
Peak Number 14 Apocynin Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.892	101.08 ng	2437600	Acenaphthene-d10	9.951

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Apocynin	166	C9H10O3	000498-02-2	96
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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TIC Library : C:\Database\NIST20.L
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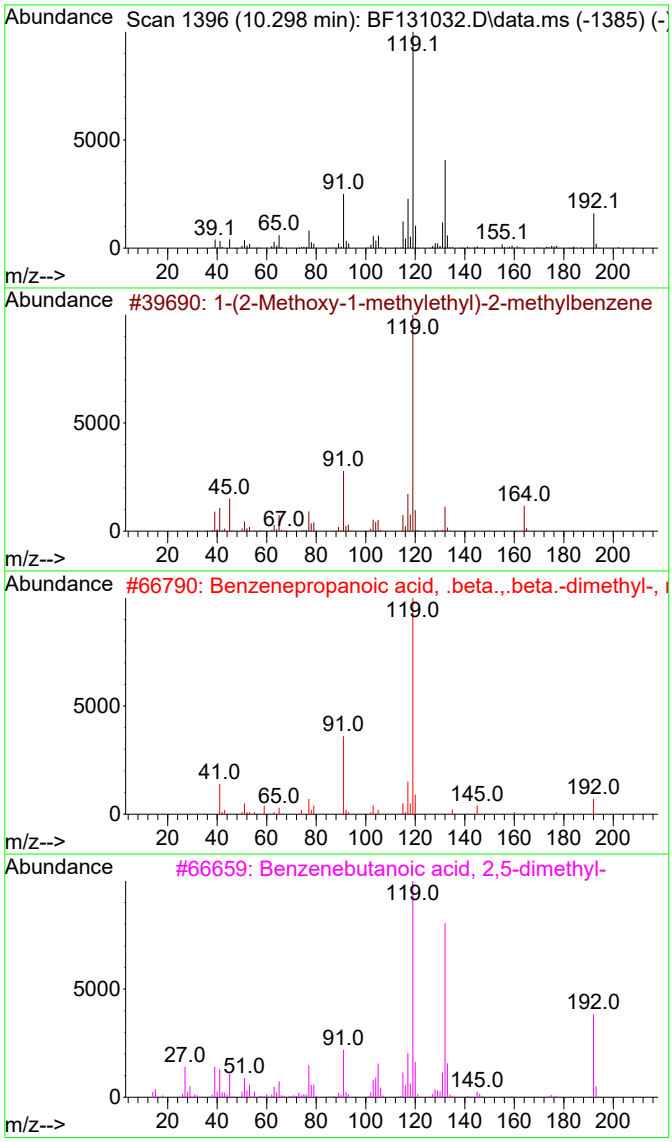
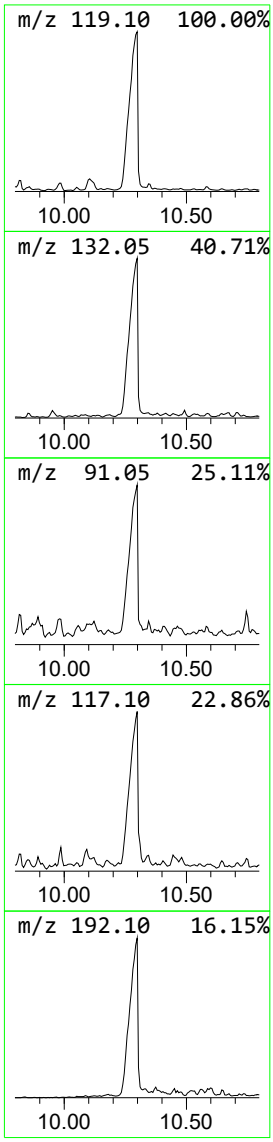
Peak Number 15 unknown10.298 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.298	184.24 ng	4443120	Acenaphthene-d10	9.951

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(2-Methoxy-1-methylethyl)-2-me...	164	C11H16O	1000210-02-1	47
2	Benzenepropanoic acid, .beta.,.b...	192	C12H16O2	025080-84-6	47
3	Benzenebutanoic acid, 2,5-dimethyl-	192	C12H16O2	001453-06-1	45
4	o-Cymene	134	C10H14	000527-84-4	43
5	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	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

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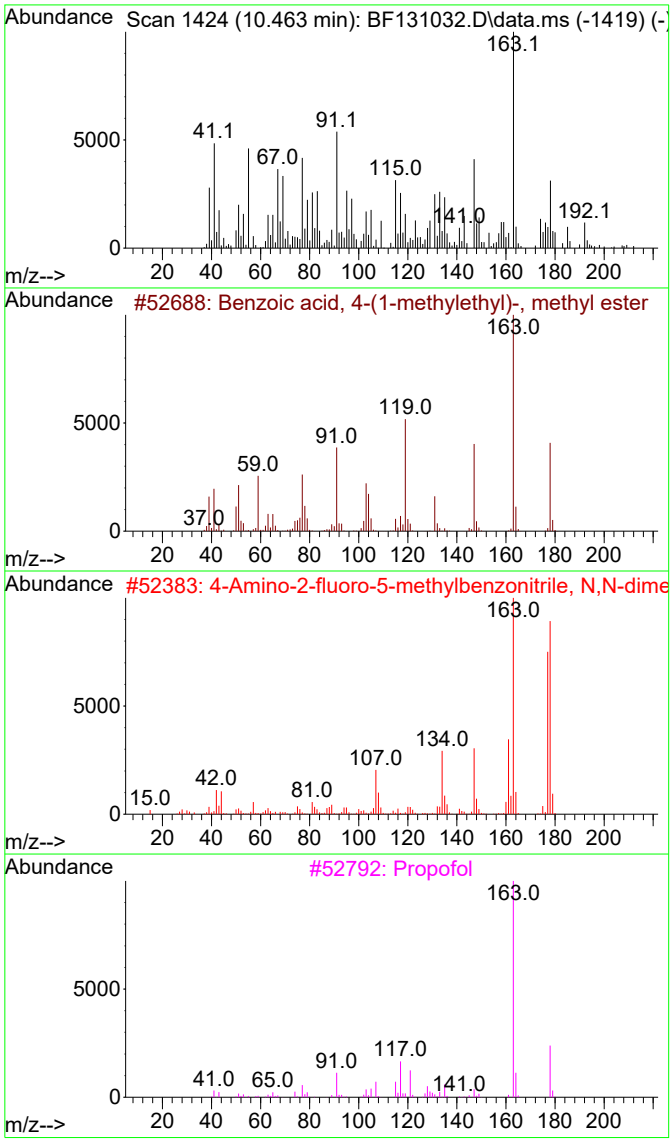
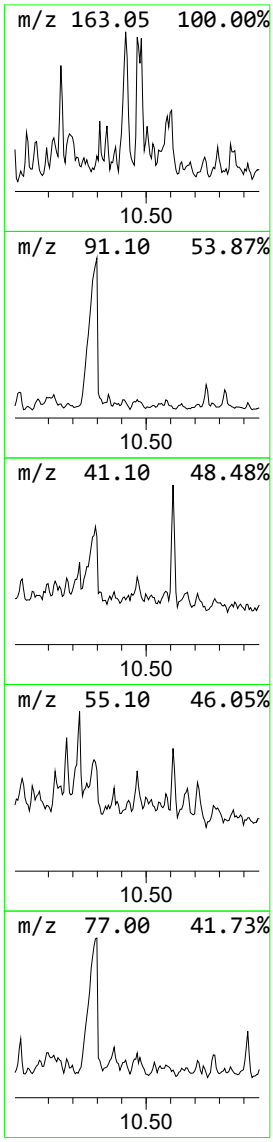
Peak Number 16 Benzoic acid, 4-(1-methylet... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.463	22.63 ng	545731	Acenaphthene-d10	9.951

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 4-(1-methylethyl)-...	178	C11H14O2	020185-55-1	55
2	4-Amino-2-fluoro-5-methylbenzoni...	178	C10H11FN2	1000511-36-7	43
3	Propofol	178	C12H18O	002078-54-8	41
4	Benzene, 1-(1-hydroxyethyl)-4-is...	178	C12H18O	040150-92-3	41
5	Benzene, 1-(1,1-dimethylethyl)-2...	178	C12H18O	000088-40-4	38





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Data File : BF131032.D
Acq On : 05 Nov 2022 22:05
Operator : CG\JU
Sample : N5340-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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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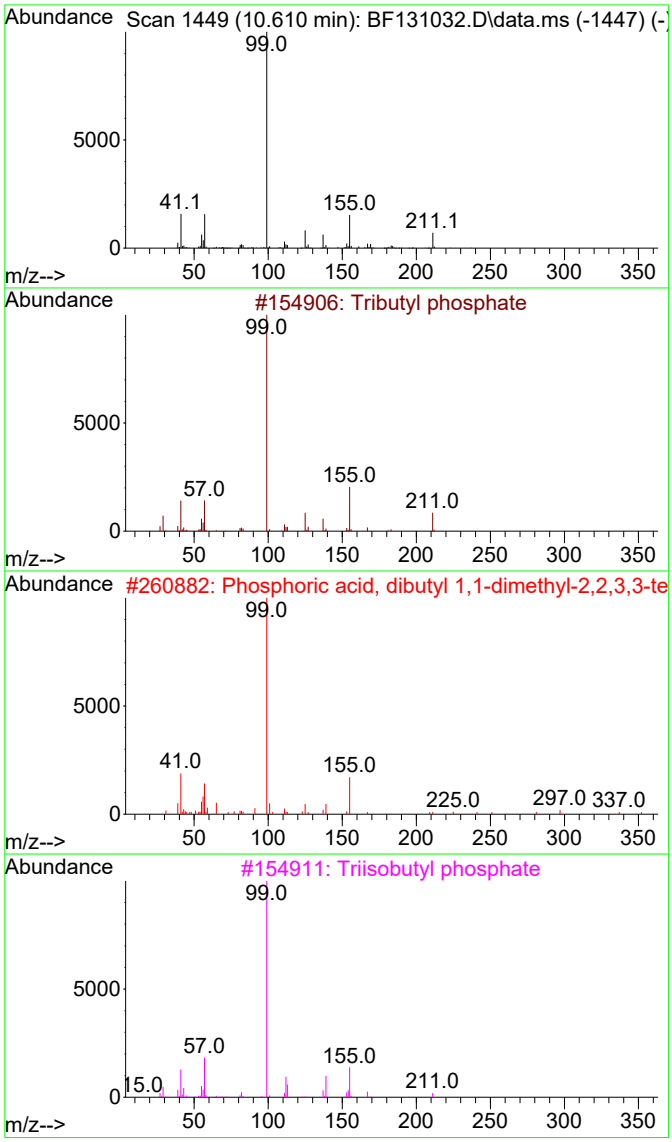
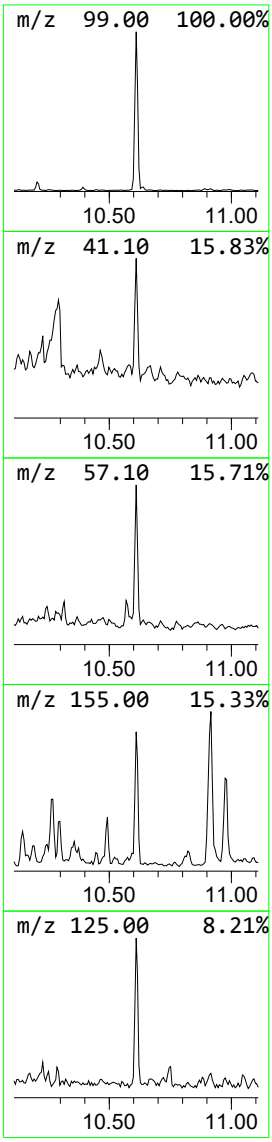
Peak Number 17 Tributyl phosphate Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.610	19.77 ng	476764	Acenaphthene-d10	9.951

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tributyl phosphate	266	C12H27O4P	000126-73-8	91
2	Phosphoric acid, dibutyl 1,1-dim...	352	C13H25F4O4P	1000298-93-9	56
3	Triisobutyl phosphate	266	C12H27O4P	000126-71-6	56
4	Phosphoric acid, dibutyl 3-trifl...	348	C14H28F3O4P	1000298-93-8	39
5	(.+/-.)-Dethiobiotin	214	C10H18N2O3	000636-20-4	36





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110522\
Data File : BF131032.D
Acq On : 05 Nov 2022 22:05
Operator : CG\JU
Sample : N5340-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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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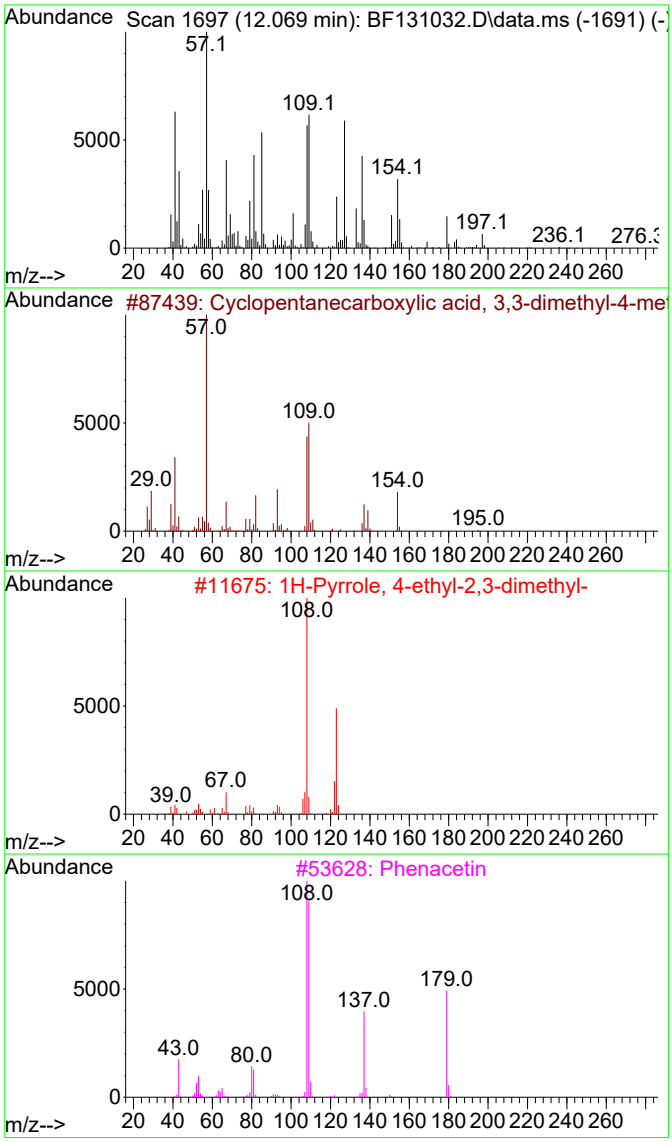
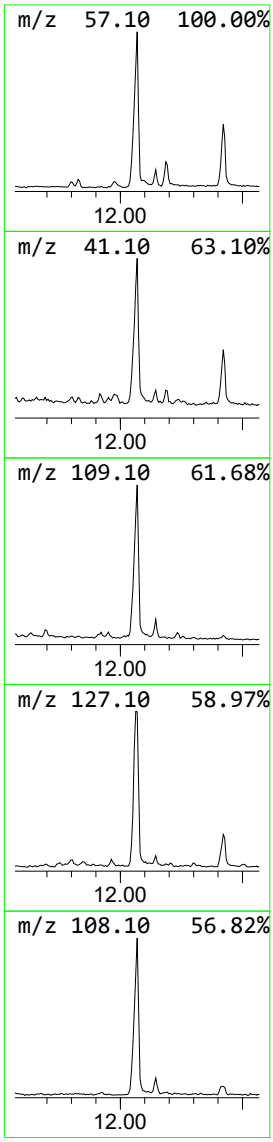
Peak Number 18 unknown12.069 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.069	72.61 ng	2113410	Phenanthrene-d10	11.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanecarboxylic acid, 3,3...	210	C13H22O2	087753-77-3	25
2	1H-Pyrrole, 4-ethyl-2,3-dimethyl-	123	C8H13N	000491-18-9	22
3	Phenacetin	179	C10H13NO2	000062-44-2	14
4	5-Fluoro-2-methylbenzoic acid	154	C8H7FO2	033184-16-6	14
5	Succinic acid, 3-chlorophenyl (2...	336	C18H21ClO4	1000391-42-1	14





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110522\
Data File : BF131032.D
Acq On : 05 Nov 2022 22:05
Operator : CG\JU
Sample : N5340-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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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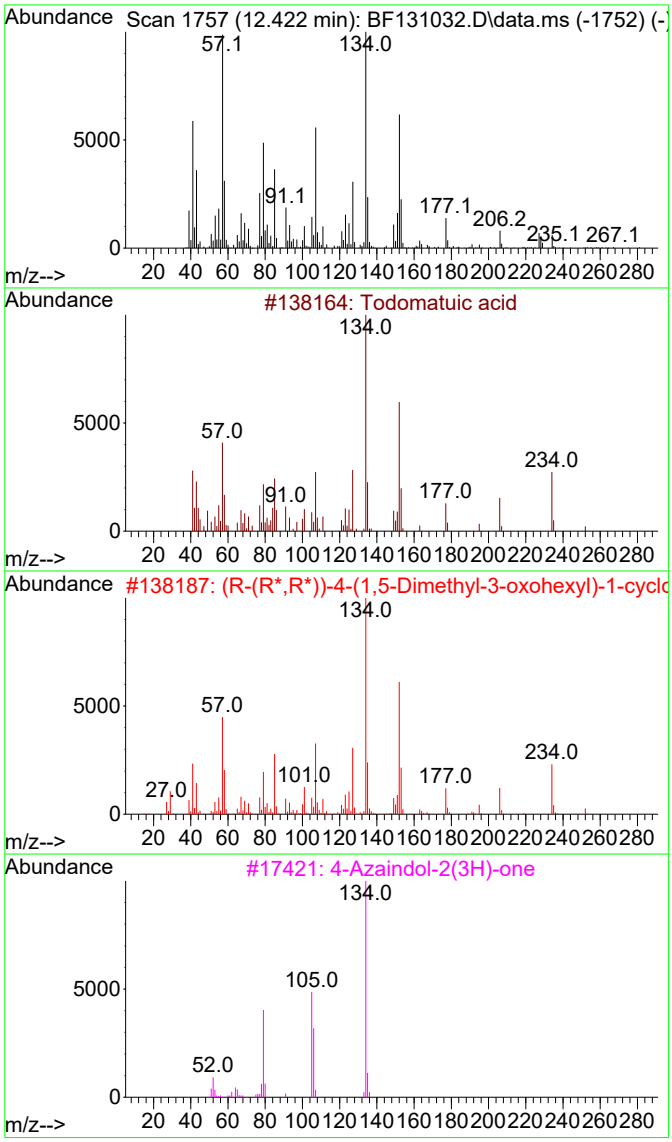
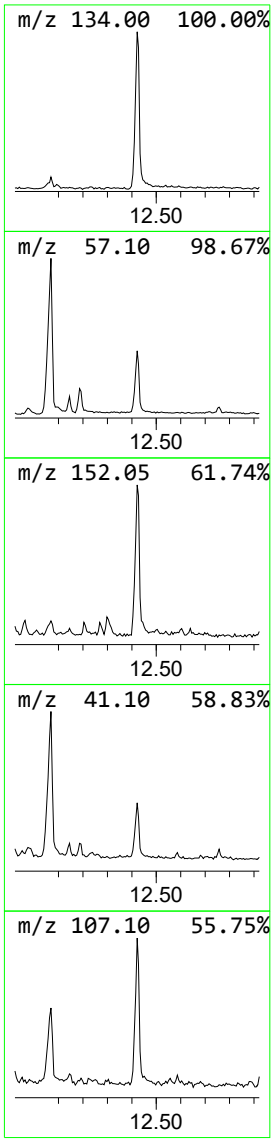
Peak Number 19 Todomatuic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.422	28.24 ng	821854	Phenanthrene-d10	11.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Todomatuic acid	252	C15H24O3	017844-07-4	64
2	(R-(R*,R*))-4-(1,5-Dimethyl-3-ox...	252	C15H24O3	006753-22-6	38
3	4-Azaindol-2(3H)-one	134	C7H6N2O	032501-05-6	38
4	1H-Purine, 6-methyl-	134	C6H6N4	002004-03-7	38
5	3-Hydroxy-4-methylbenzoic acid	152	C8H8O3	000586-30-1	30





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Data File : BF131032.D
Acq On : 05 Nov 2022 22:05
Operator : CG\JU
Sample : N5340-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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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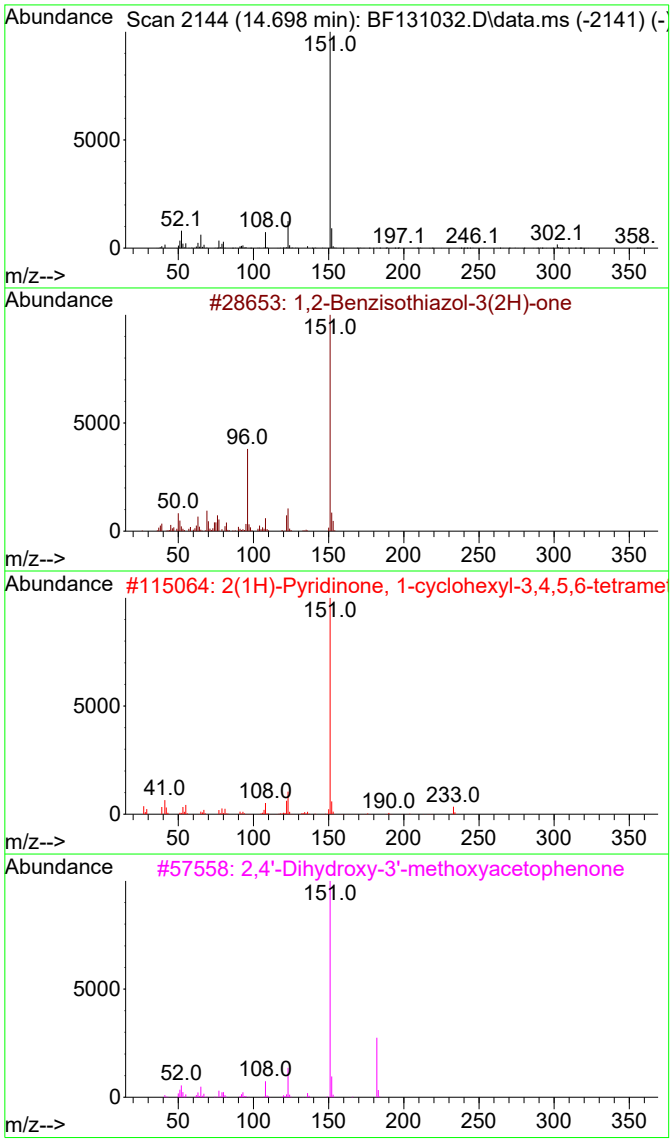
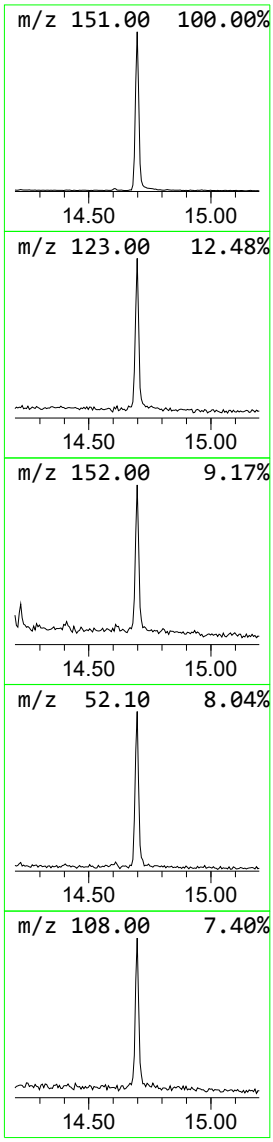
Peak Number 20 1,2-Benzisothiazol-3(2H)-one Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.698	21.70 ng	411178	Chrysene-d12	14.092

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	72
2	2(1H)-Pyridinone, 1-cyclohexyl-3...	233	C15H23NO	082754-44-7	72
3	2,4'-Dihydroxy-3'-methoxyacetoph...	182	C9H10O4	018256-48-9	64
4	Ethanone, 1-(3-hydroxy-4-methoxy...	166	C9H10O3	006100-74-9	56
5	3-Hydroxymethylbenzamide	151	C8H9NO2	126926-34-9	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110522\
Data File : BF131032.D
Acq On : 05 Nov 2022 22:05
Operator : CG\JU
Sample : N5340-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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...	2.187	62.9	ng	1763100	1	6.904	560751	20.0
1,3,5,7-Cyclooc...	5.740	23.9	ng	668851	1	6.904	560751	20.0
unknown6.963	6.963	27.3	ng	765205	1	6.904	560751	20.0
1-Heptene, 3-me...	6.975	39.9	ng	1119630	1	6.904	560751	20.0
Heptanoic acid	7.369	30.9	ng	867117	1	6.904	560751	20.0
(+)-2-Bornanone	7.940	31.8	ng	2128250	2	8.187	1337200	20.0
endo-Borneol	8.116	75.3	ng	5037520	2	8.187	1337200	20.0
Benzoic acid, 2...	9.104	20.5	ng	494962	3	9.951	482318	20.0
Benzoic acid, 2...	9.139	18.5	ng	445175	3	9.951	482318	20.0
Benzaldehyde, 4...	9.175	22.3	ng	538035	3	9.951	482318	20.0
Vanillin	9.445	226.8	ng	5469000	3	9.951	482318	20.0
4-tert-Butyl-2-...	9.716	26.8	ng	646560	3	9.951	482318	20.0
Benzoic acid, 2...	9.816	20.8	ng	502068	3	9.951	482318	20.0
Apocynin	9.892	101.1	ng	2437600	3	9.951	482318	20.0
unknown10.298	10.298	184.2	ng	4443120	3	9.951	482318	20.0
Benzoic acid, 4...	10.463	22.6	ng	545731	3	9.951	482318	20.0
Tributyl phosphate	10.610	19.8	ng	476764	3	9.951	482318	20.0
unknown12.069	12.069	72.6	ng	2113410	4	11.445	582093	20.0
Todomatuic acid	12.422	28.2	ng	821854	4	11.445	582093	20.0
1,2-Benzisothia...	14.698	21.7	ng	411178	5	14.092	379031	20.0