LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032922\
Data File : BF127563.D
Acq On : 29 Mar 2022 14:10
Operator : CG\JU
Sample : N2154-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5

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-BF032122.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127563.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.281	164	169	182	rBV	56855	113240	1.96%	0.236%
2	5.234	490	501	509	rBV5	47184	171478	2.96%	0.357%
3	5.457	537	539	554	rBV	706229	939881	16.23%	1.958%
4	5.669	571	575	580	rVB4	40834	72135	1.25%	0.150%
5	6.098	645	648	652	rBV2	47952	58684	1.01%	0.122%
6	6.487	711	714	721	rBV	352325	686677	11.86%	1.431%
7	6.645	738	741	744	rBV2	60828	67535	1.17%	0.141%
8	6.710	749	752	759	rVB6	74236	114205	1.97%	0.238%
9	6.828	768	772	777	rBV	533798	527580	9.11%	1.099%
10	6.898	777	784	789	rBV3	179689	335502	5.79%	0.699%
11	7.098	813	818	821	rBV	104538	118886	2.05%	0.248%
12	7.169	827	830	836	rVB3	77082	89510	1.55%	0.187%
13	7.222	836	839	841	rBV2	97470	108636	1.88%	0.226%
14	7.281	841	849	852	rVV3	265252	434692	7.51%	0.906%
15	7.310	852	854	860	rVB2	125693	135549	2.34%	0.282%
16	7.404	863	870	872	rBV	1937089	1994715	34.45%	4.156%
17	7.422	872	873	877	rVB	785052	606744	10.48%	1.264%
18	7.522	885	890	893	rBV5	70545	111483	1.93%	0.232%
19	7.581	893	900	903	rBV4	229518	307048	5.30%	0.640%
20	7.651	909	912	916	rBV2	140759	227034	3.92%	0.473%
21	7.698	916	920	923	rVB2	217471	241340	4.17%	0.503%
22	7.734	923	926	930	rVB3	124559	168103	2.90%	0.350%
23	7.798	931	937	939	rBV	114749	138253	2.39%	0.288%
24	7.834	939	943	944	rBV3	148607	191342	3.30%	0.399%
25	7.863	944	948	951	rVB	1290881	1242611	21.46%	2.589%
26	7.922	953	958	959	rBV2	321858	435417	7.52%	0.907%
27	8.028	973	976	982	rBV3	726294	1137063	19.64%	2.369%
28	8.081	982	985	988	rVV2	165593	211609	3.65%	0.441%
29	8.116	988	991	993	rVV	755135	711364	12.29%	1.482%
30	8.145	993	996	999	rVV	2610404	2399023	41.43%	4.999%
31	8.210	1005	1007	1011	rVB3	107193	100124	1.73%	0.209%
32	8.251	1011	1014	1016	rBV2	442768	467808	8.08%	0.975%
33	8.269	1016	1017	1021	rVB2	390768	274253	4.74%	0.571%
34	8.310	1021	1024	1027	rVB4	65170	75397	1.30%	0.157%
35	8.357	1027	1032	1039	rVB7	294450	565766	9.77%	1.179%
36	8.410	1039	1041	1042	rBV	63964	62633	1.08%	0.131%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032922\
Data File : BF127563.D
Acq On : 29 Mar 2022 14:10
Operator : CG\JU
Sample : N2154-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5

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-BF032122.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	8.451	1045	1048	1052	rVB4	82943	114172	1.97%	0.238%
38	8.492	1053	1055	1058	rBV2	131493	142099	2.45%	0.296%
39	8.528	1058	1061	1063	rBV	228084	209550	3.62%	0.437%
40	8.551	1063	1065	1066	rVV	163617	140669	2.43%	0.293%
41	8.575	1066	1069	1074	rVV5	212049	381205	6.58%	0.794%
42	8.610	1074	1075	1081	rVB3	139631	145159	2.51%	0.302%
43	8.663	1081	1084	1087	rVB3	112561	108408	1.87%	0.226%
44	8.692	1087	1089	1092	rBV2	91690	90978	1.57%	0.190%
45	8.722	1092	1094	1096	rBV2	130314	106837	1.85%	0.223%
46	8.745	1096	1098	1101	rVB4	108046	87600	1.51%	0.183%
47	8.792	1104	1106	1111	rVB4	128091	167591	2.89%	0.349%
48	8.839	1111	1114	1118	rBV5	151491	278682	4.81%	0.581%
49	8.881	1118	1121	1123	rVB	309940	264039	4.56%	0.550%
50	8.916	1123	1127	1134	rVB4	258853	454281	7.85%	0.947%
51	8.986	1134	1139	1141	rBV4	261523	412058	7.12%	0.859%
52	9.016	1141	1144	1148	rVB3	252523	312975	5.41%	0.652%
53	9.057	1148	1151	1153	rBV3	190296	178562	3.08%	0.372%
54	9.092	1153	1157	1161	rBV4	256704	317971	5.49%	0.663%
55	9.133	1162	1164	1166	rBV2	113698	100757	1.74%	0.210%
56	9.192	1170	1174	1177	rVB	3190930	2833202	48.93%	5.903%
57	9.257	1182	1185	1186	rBV2	96782	76954	1.33%	0.160%
58	9.292	1186	1191	1193	rBV	558474	710210	12.27%	1.480%
59	9.357	1197	1202	1205	rBV	2000764	2295245	39.64%	4.782%
60	9.428	1212	1214	1217	rVB3	117406	104983	1.81%	0.219%
61	9.481	1220	1223	1224	rVV3	99240	89040	1.54%	0.186%
62	9.498	1224	1226	1227	rVV2	115147	103825	1.79%	0.216%
63	9.539	1231	1233	1238	rVV3	318044	502859	8.68%	1.048%
64	9.610	1242	1245	1249	rVV3	202633	330649	5.71%	0.689%
65	9.645	1249	1251	1256	rVB	393629	379707	6.56%	0.791%
66	9.739	1265	1267	1271	rVB3	151913	164416	2.84%	0.343%
67	9.781	1272	1274	1276	rBV2	66784	67472	1.17%	0.141%
68	9.810	1276	1279	1282	rVV	702300	628160	10.85%	1.309%
69	9.839	1282	1284	1287	rVB2	191954	164863	2.85%	0.344%
70	9.875	1287	1290	1293	rBV	688839	619154	10.69%	1.290%
71	10.104	1327	1329	1335	rVB	579385	600051	10.36%	1.250%
72	10.228	1337	1350	1354	rBV	2210853	5790337	100.00%	12.065%
73	10.480	1387	1393	1395	rBV4	228367	365120	6.31%	0.761%
74	10.504	1395	1397	1405	rVB3	220511	245308	4.24%	0.511%
75	10.669	1422	1425	1429	rVB	1457621	1311560	22.65%	2.733%
76	10.757	1438	1440	1446	rVB2	88672	82056	1.42%	0.171%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032922\
Data File : BF127563.D
Acq On : 29 Mar 2022 14:10
Operator : CG\JU
Sample : N2154-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5

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-BF032122.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	10.998	1479	1481	1488	rVB2	158088	240786	4.16%	0.502%
78	11.251	1522	1524	1529	rVB3	203915	198880	3.43%	0.414%
79	11.298	1530	1532	1535	rBV2	81692	78516	1.36%	0.164%
80	11.369	1540	1544	1546	rVV	564214	510623	8.82%	1.064%
81	11.722	1600	1604	1606	rBV2	224753	301565	5.21%	0.628%
82	11.745	1606	1608	1611	rVB	372749	282169	4.87%	0.588%
83	11.898	1631	1634	1641	rVB3	132475	197921	3.42%	0.412%
84	11.992	1643	1650	1653	rBV	1845682	2707200	46.75%	5.641%
85	12.069	1660	1663	1668	rVB	244892	196592	3.40%	0.410%
86	12.122	1668	1672	1676	rBV	465614	556129	9.60%	1.159%
87	12.357	1706	1712	1725	rBV	1042692	1492641	25.78%	3.110%
88	12.674	1764	1766	1775	rVB4	105296	120530	2.08%	0.251%
89	12.874	1798	1800	1803	rVB	104332	82272	1.42%	0.171%
90	12.951	1809	1813	1816	rVB	1982840	1717050	29.65%	3.578%
91	13.333	1875	1878	1884	rBV	373416	406434	7.02%	0.847%
92	13.816	1957	1960	1963	rVV	192706	185689	3.21%	0.387%
93	13.845	1963	1965	1970	rVB2	136024	136750	2.36%	0.285%
94	14.016	1992	1994	1997	rBV	490133	431399	7.45%	0.899%
95	14.045	1997	1999	2007	rVB2	114916	144390	2.49%	0.301%
96	14.615	2093	2096	2104	rVB	315653	345776	5.97%	0.720%
97	15.504	2243	2247	2256	rVB	400199	538844	9.31%	1.123%

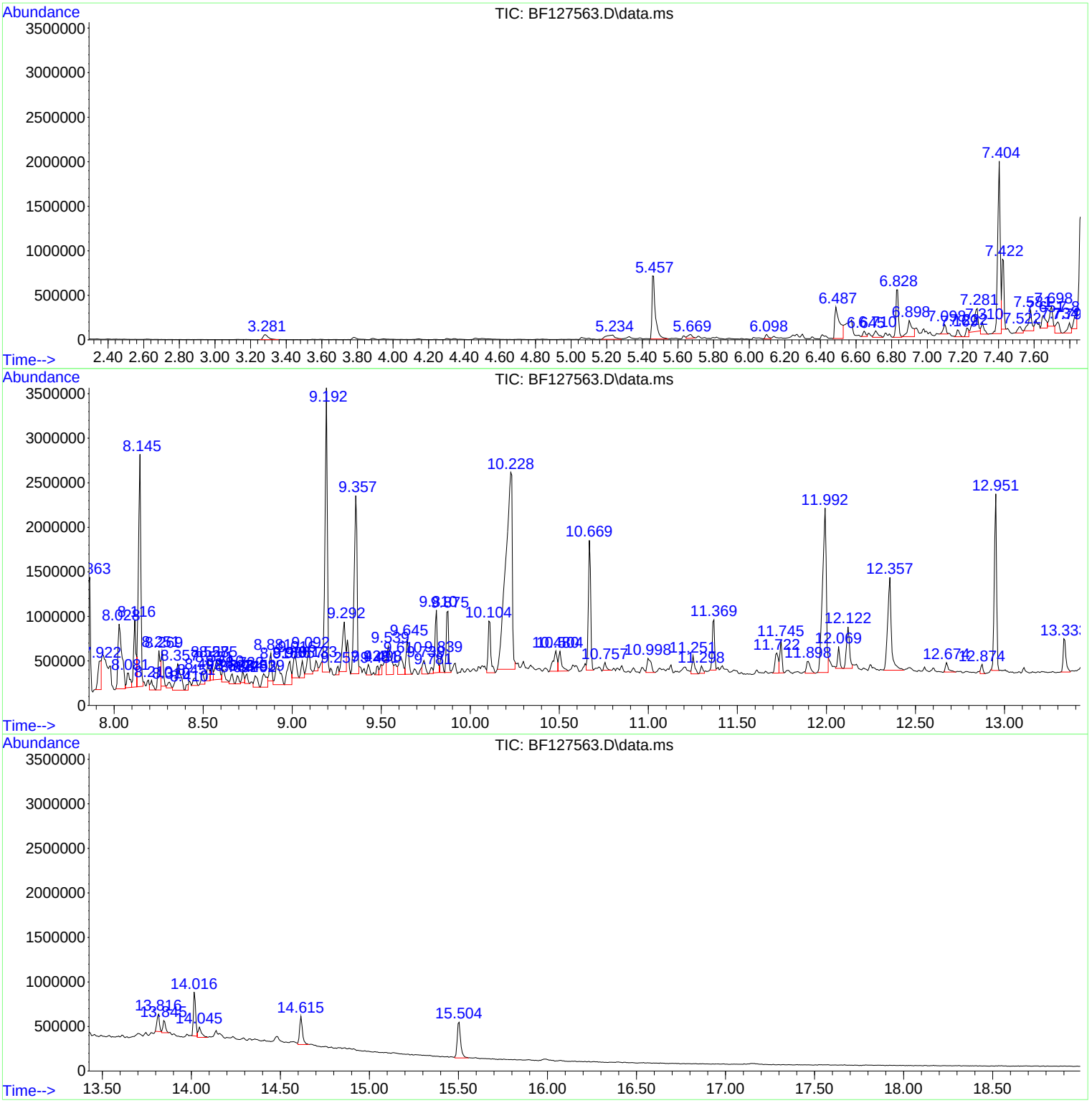
Sum of corrected areas: 47994240

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032922\
Data File : BF127563.D
Acq On : 29 Mar 2022 14:10
Operator : CG\JU
Sample : N2154-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.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\BF032922\
Data File : BF127563.D
Acq On : 29 Mar 2022 14:10
Operator : CG\JU
Sample : N2154-01
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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

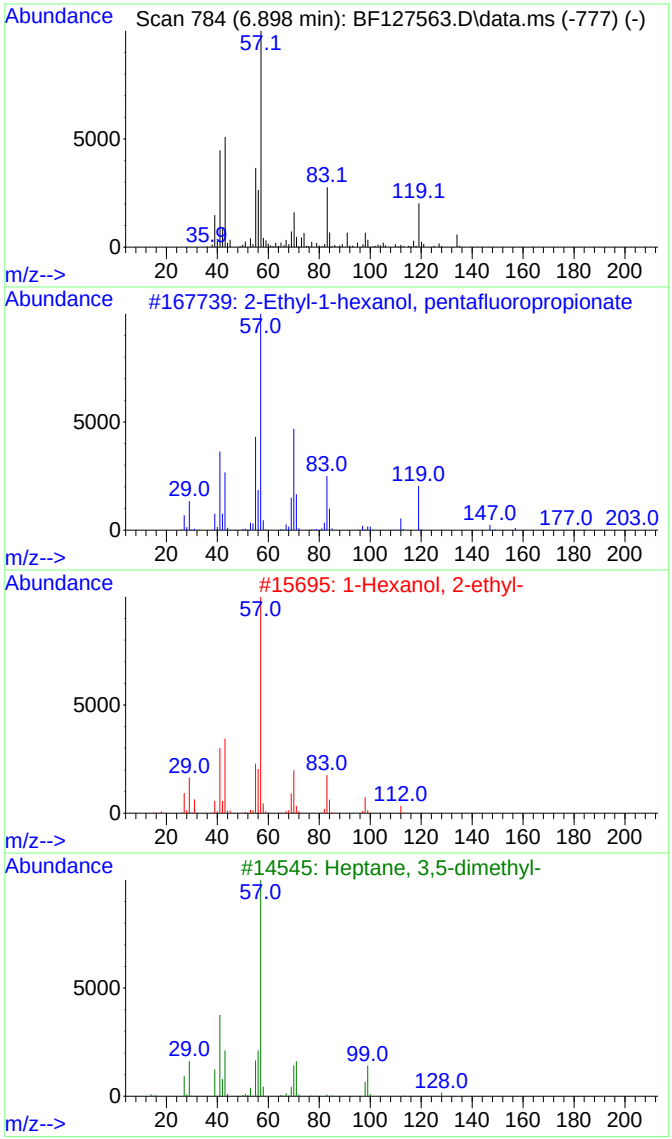
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

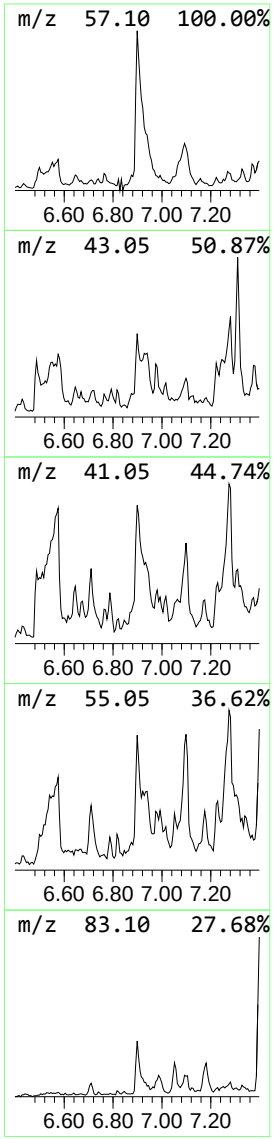
****

Peak Number 1 unknown6.898 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.898	12.72 ng	335502	1,4-Dichlorobenzene-d4	6.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Ethyl-1-hexanol, pentafluoropr...	276	C11H17F5O2	959012-82-9	40
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	38
3	Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	38
4	1-Pentene, 4,4-dimethyl-	98	C7H14	000762-62-9	38
5	Silane, trichlorodocosyl-	442	C22H45Cl3Si	007325-84-0	37





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032922\
Data File : BF127563.D
Acq On : 29 Mar 2022 14:10
Operator : CG\JU
Sample : N2154-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

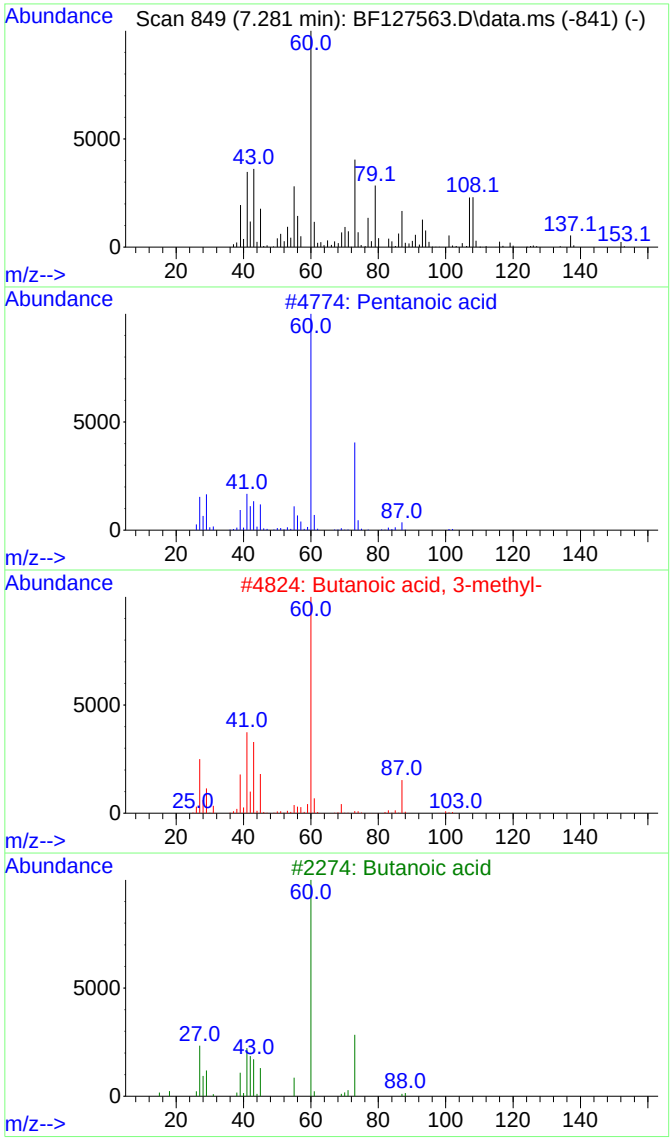
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

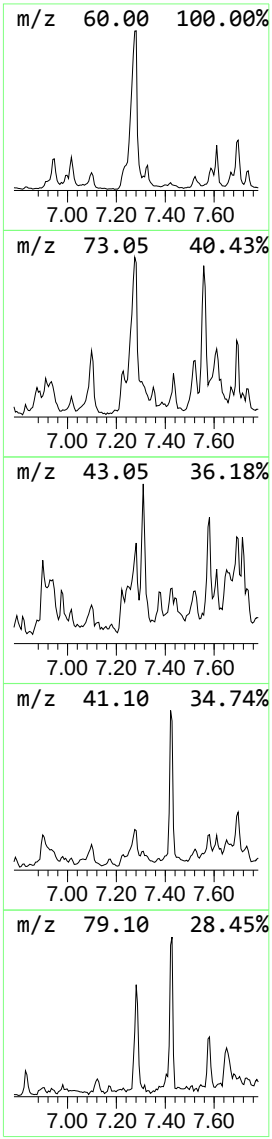
****

Peak Number 2 unknown7.281 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.281	16.48 ng	434692	1,4-Dichlorobenzene-d4	6.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanoic acid	102	C5H10O2	000109-52-4	49
2	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	46
3	Butanoic acid	88	C4H8O2	000107-92-6	43
4	Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	43
5	Hexanoic acid, 6-bromo-	194	C6H11BrO2	004224-70-8	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032922\
Data File : BF127563.D
Acq On : 29 Mar 2022 14:10
Operator : CG\JU
Sample : N2154-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5

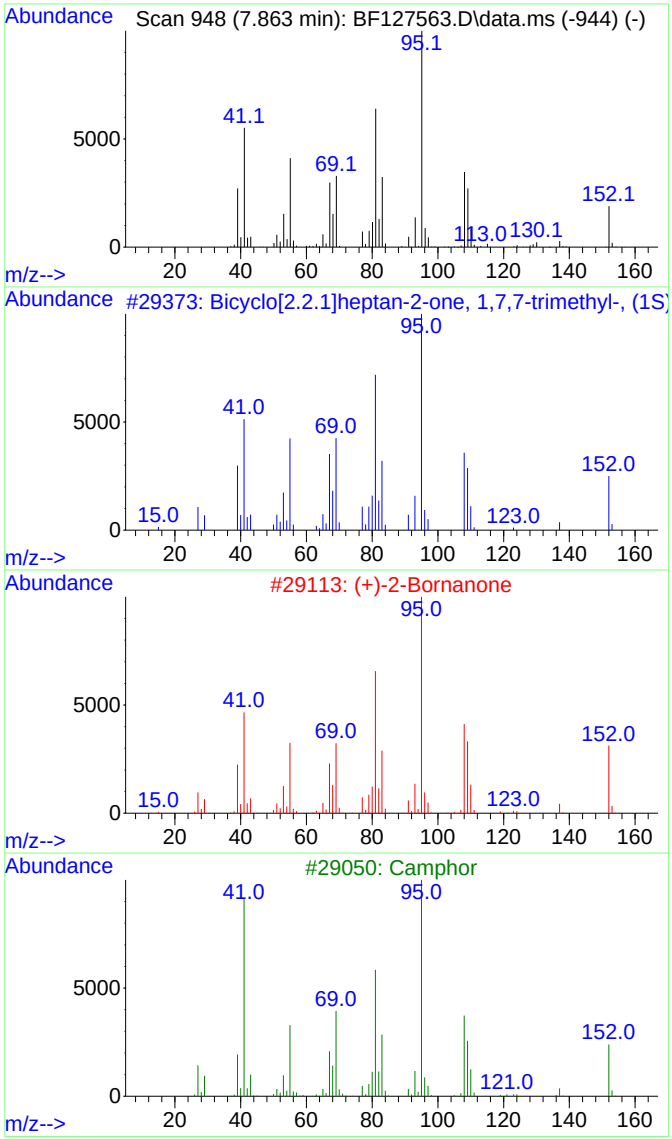
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

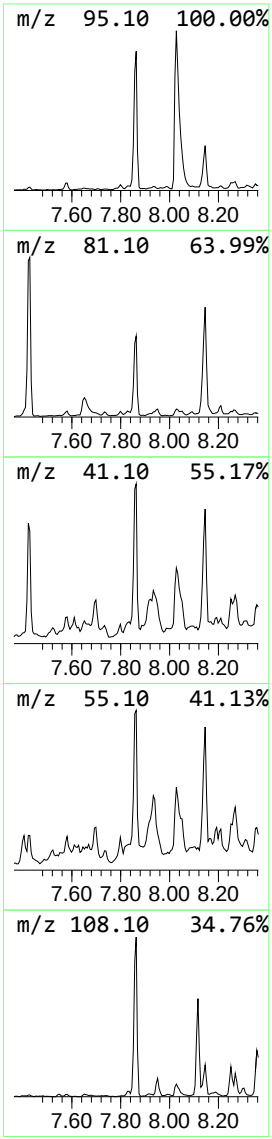
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.863	34.94 ng	1242610	Naphthalene-d8	8.116

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	96
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





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032922\
Data File : BF127563.D
Acq On : 29 Mar 2022 14:10
Operator : CG\JU
Sample : N2154-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

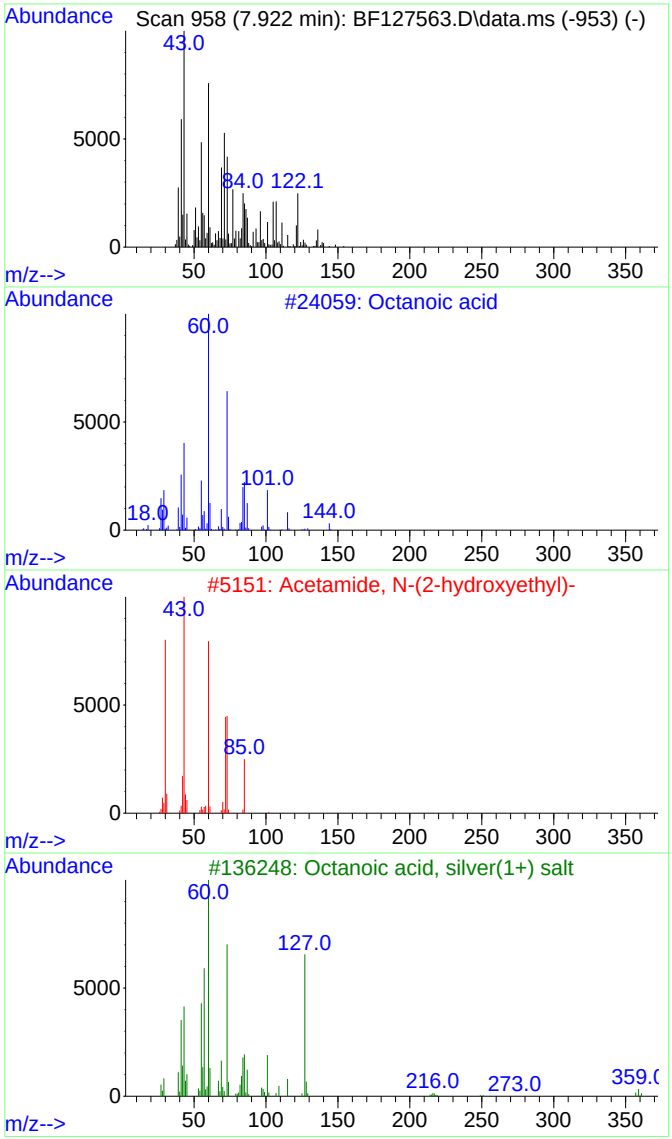
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

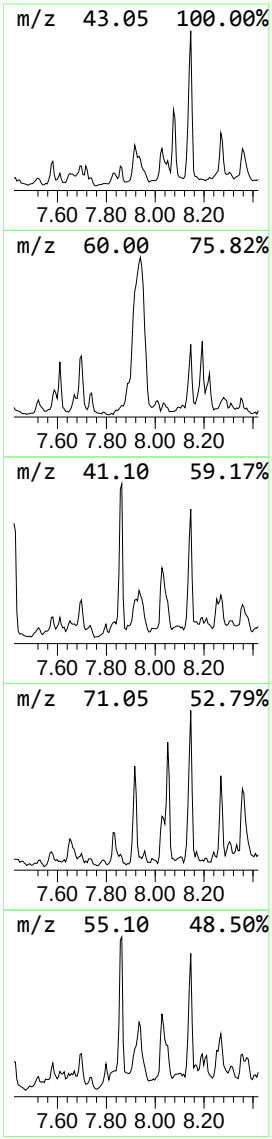
****

Peak Number 4 unknown7.922 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.922	12.24 ng	435417	Naphthalene-d8	8.116

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanoic acid	144	C8H16O2	000124-07-2	35
2	Acetamide, N-(2-hydroxyethyl)-	103	C4H9NO2	000142-26-7	27
3	Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	27
4	Heptanoic acid	130	C7H14O2	000111-14-8	27
5	Pentanoic acid	102	C5H10O2	000109-52-4	14





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032922\
Data File : BF127563.D
Acq On : 29 Mar 2022 14:10
Operator : CG\JU
Sample : N2154-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

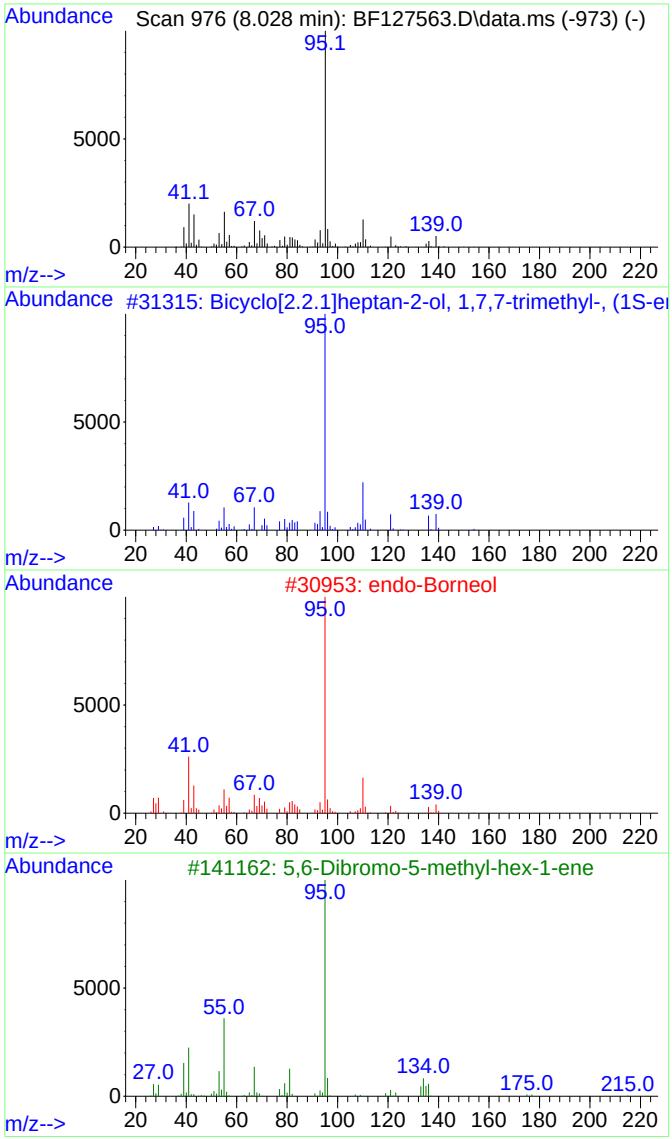
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

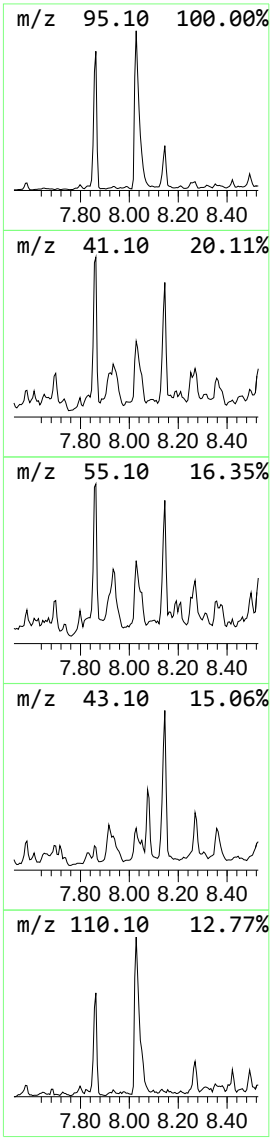
****

Peak Number 5 Bicyclo[2.2.1]heptan-2-ol, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.028	31.97 ng	1137060	Naphthalene-d8	8.116

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]heptan-2-ol, 1,7,7...	154	C10H18O	000464-45-9	83
2	endo-Borneol	154	C10H18O	000507-70-0	78
3	5,6-Dibromo-5-methyl-hex-1-ene	254	C7H12Br2	1000192-24-6	64
4	1,4-Pentadiene, 2,3,4-trimethyl-	110	C8H14	072014-90-5	64
5	Furan, 2-ethyl-5-methyl-	110	C7H10O	001703-52-2	59





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Acq On : 29 Mar 2022 14:10
Operator : CG\JU
Sample : N2154-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

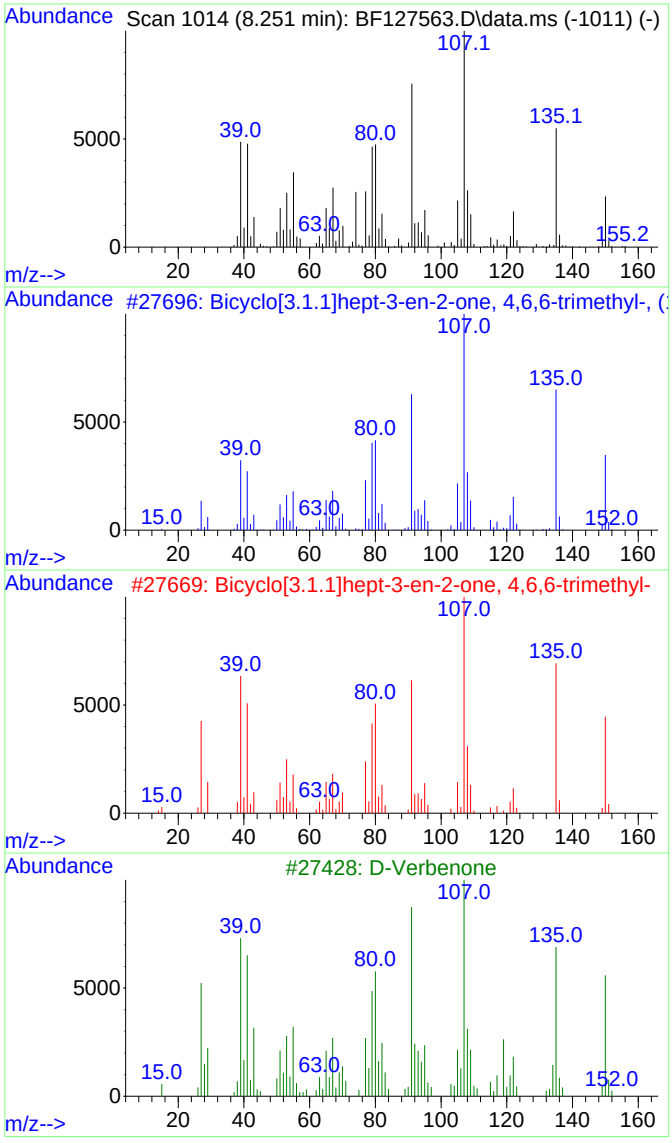
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

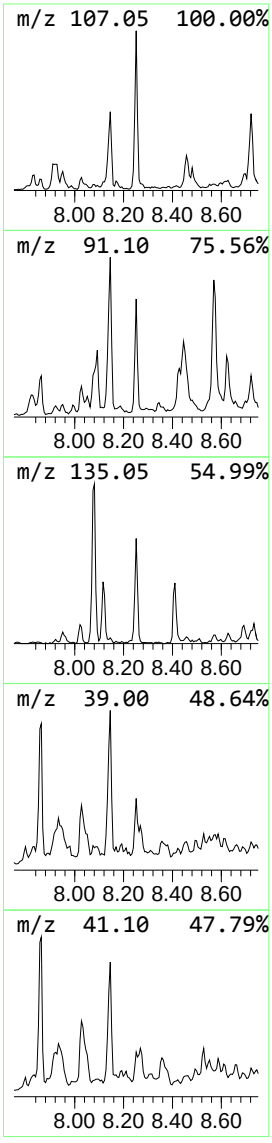
****

Peak Number 6 Bicyclo[3.1.1]hept-3-en-2-o... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.251	13.15 ng	467808	Naphthalene-d8	8.116

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[3.1.1]hept-3-en-2-one, 4...	150	C10H14O	001196-01-6	98
2	Bicyclo[3.1.1]hept-3-en-2-one, 4...	150	C10H14O	000080-57-9	93
3	D-Verbenone	150	C10H14O	018309-32-5	90
4	Bicyclo[3.1.1]hept-2-en-6-one, 2...	150	C10H14O	000473-06-3	90
5	1,3-Cyclopentadiene, 1,2,5,5-tet...	122	C9H14	004249-12-1	50





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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

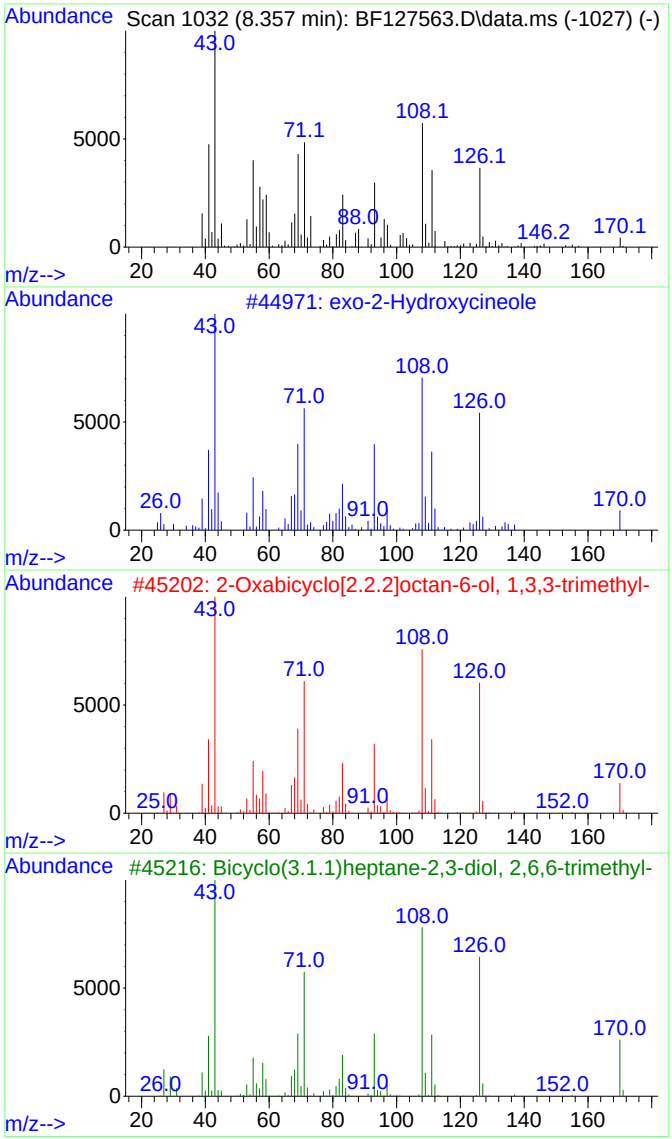
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

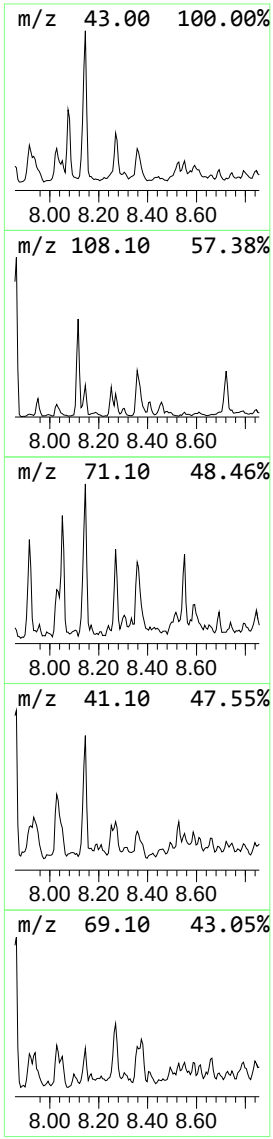
****

Peak Number 7 exo-2-Hydroxycineole Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.357	15.91 ng	565766	Naphthalene-d8	8.116

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	exo-2-Hydroxycineole	170	C10H18O2	092999-78-5	94
2	2-Oxabicyclo[2.2.2]octan-6-ol, 1...	170	C10H18O2	018679-48-6	93
3	Bicyclo(3.1.1)heptane-2,3-diol, ...	170	C10H18O2	053404-49-2	76
4	5-Hepten-2-one, 6-methyl-	126	C8H14O	000110-93-0	35
5	2-Oxabicyclo[2.2.2]octan-6-ol, 1...	212	C12H20O3	057709-95-2	32





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Sample : N2154-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

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

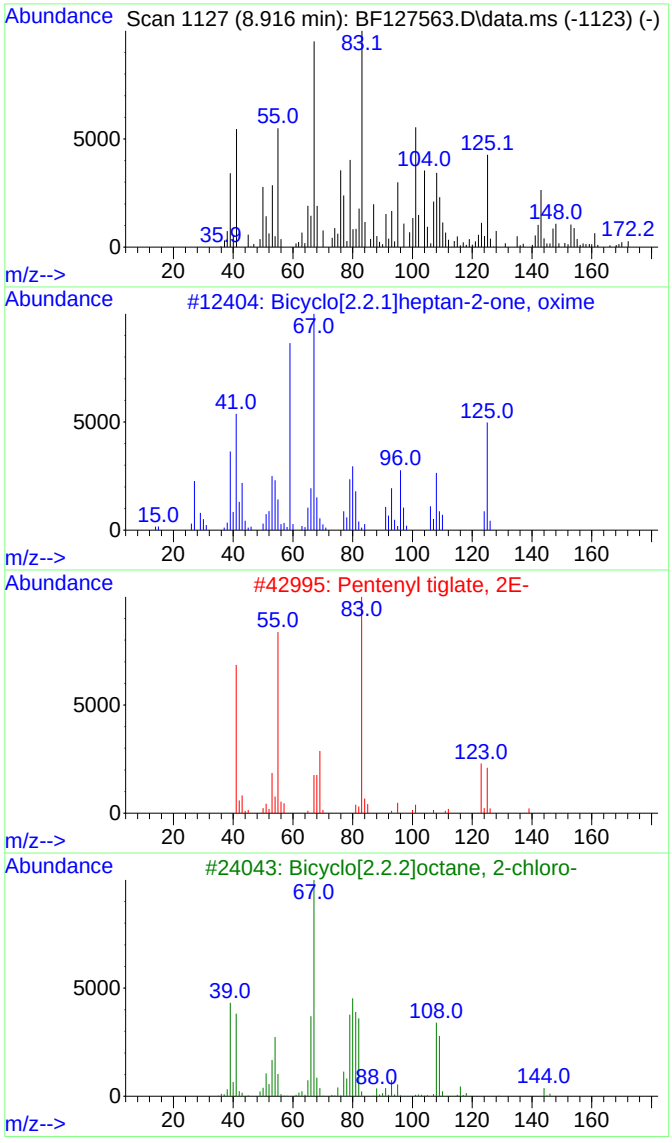
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

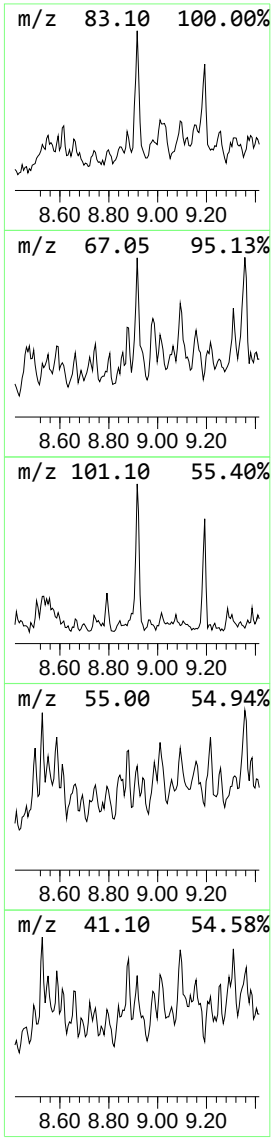
****

Peak Number 8 unknown8.916 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.916	12.77 ng	454281	Naphthalene-d8	8.116

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]heptan-2-one, oxime	125	C7H11NO	1000142-10-9	25
2	Pentenyl tiglate, 2E-	168	C10H16O2	1000383-58-8	22
3	Bicyclo[2.2.2]octane, 2-chloro-	144	C8H13Cl	033649-79-5	22
4	3-Cyclopentylpropionic acid, cyc...	210	C13H22O2	1000293-36-7	22
5	Pyrazine, 2,3-dimethyl-	108	C6H8N2	005910-89-4	18





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Sample : N2154-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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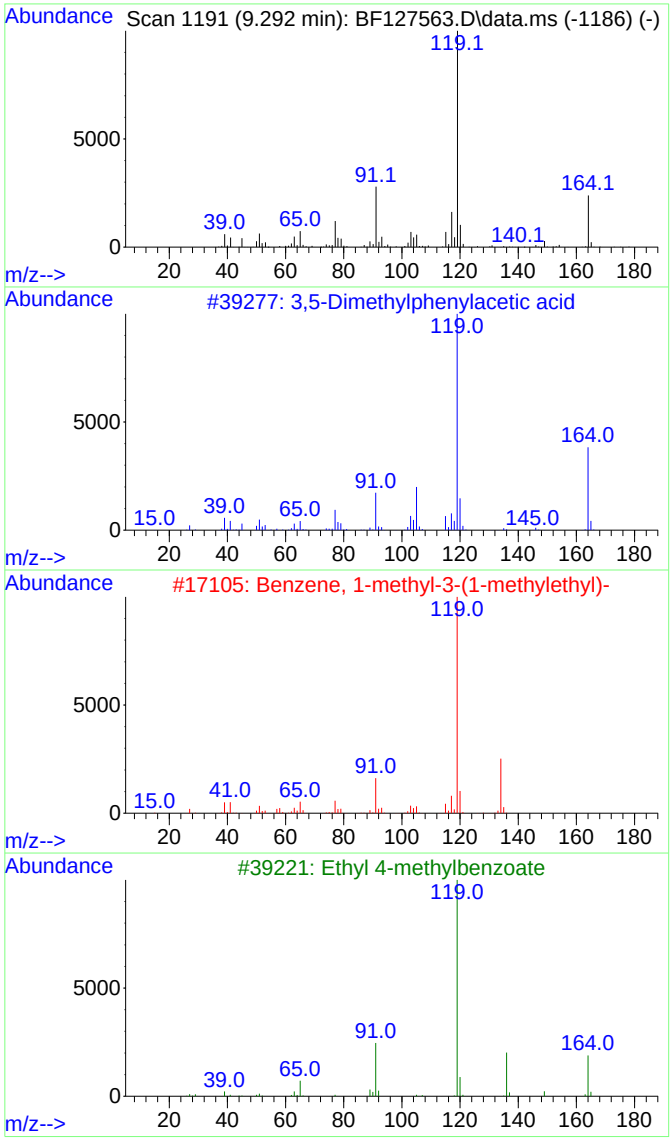
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

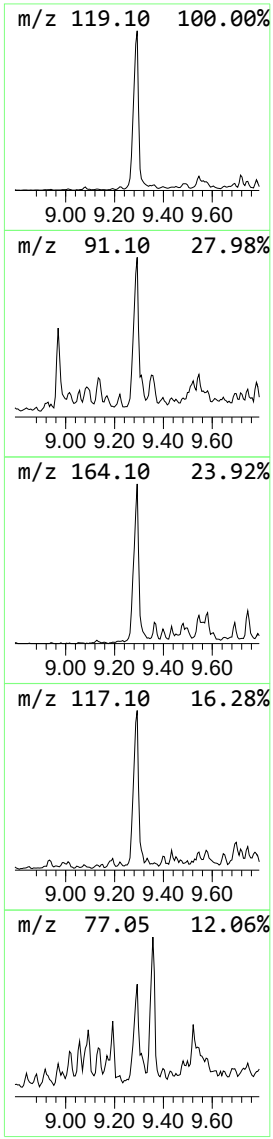
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 3,5-Dimethylphenylacetic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.292	22.94 ng	710210	Acenaphthene-d10	9.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-Dimethylphenylacetic acid	164	C10H12O2	042288-46-0	91
2	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	64
3	Ethyl 4-methylbenzoate	164	C10H12O2	000094-08-6	64
4	o-Cymene	134	C10H14	000527-84-4	64
5	p-Cymene	134	C10H14	000099-87-6	64





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Operator : CG\JU
Sample : N2154-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.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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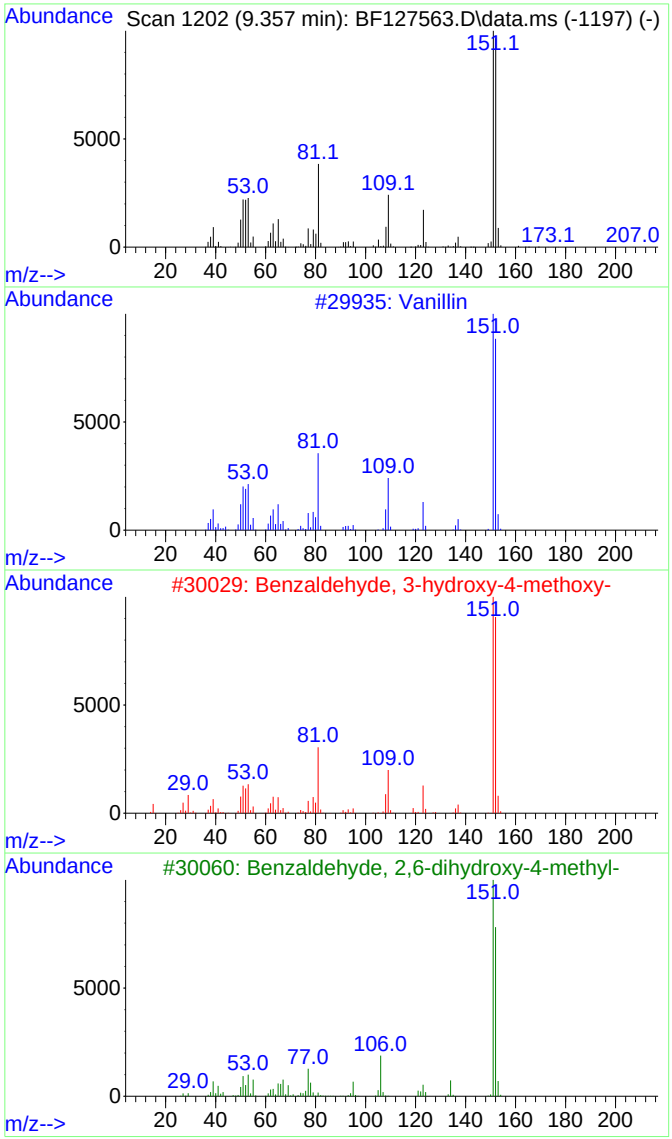
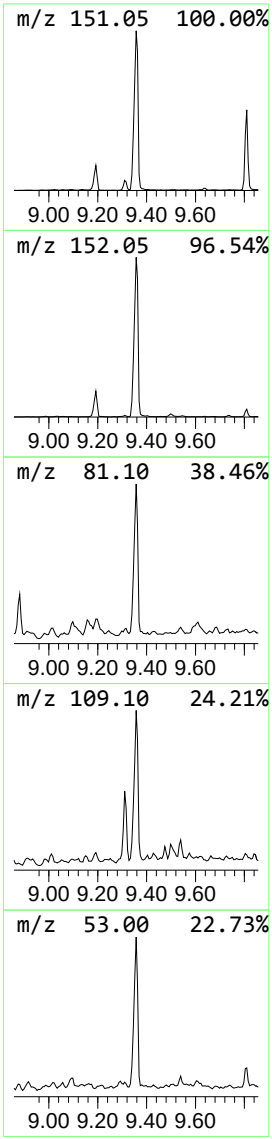
Peak Number 10 Vanillin Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.357	74.14 ng	2295250	Acenaphthene-d10	9.875

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	Benzaldehyde, 2,6-dihydroxy-4-me...	152	C8H8O3	000526-37-4	47
4	Benzaldehyde, 2-hydroxy-4-methoxy-	152	C8H8O3	000673-22-3	46
5	Benzaldehyde, 2,4-dihydroxy-6-me...	152	C8H8O3	000487-69-4	43





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Misc :
ALS Vial : 8 Sample Multiplier: 1

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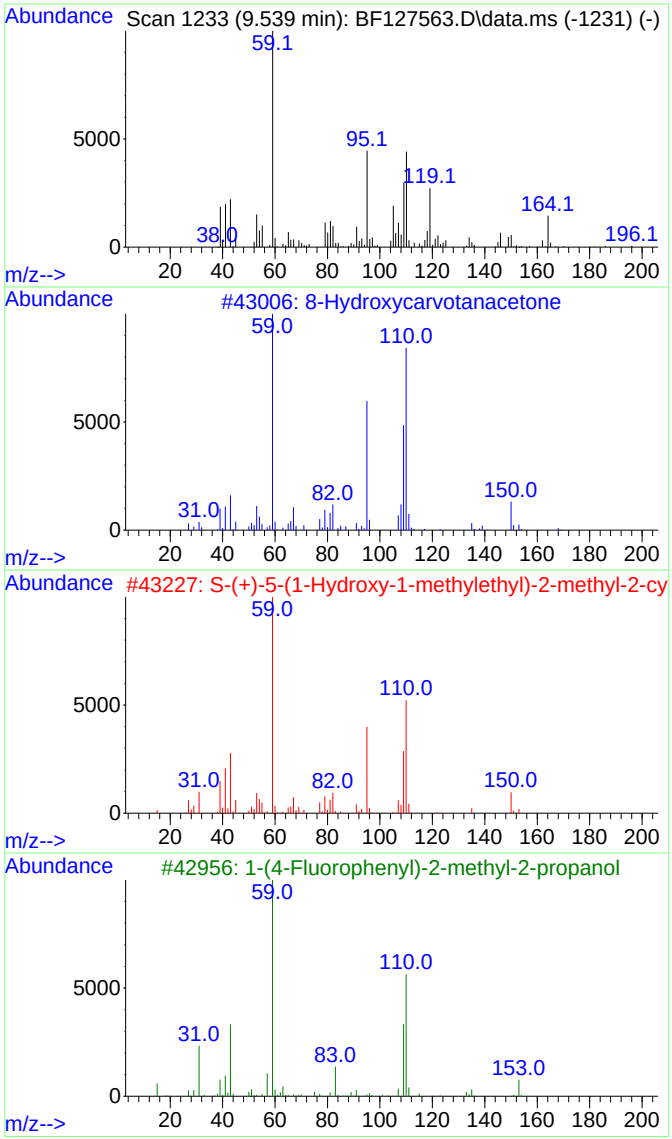
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

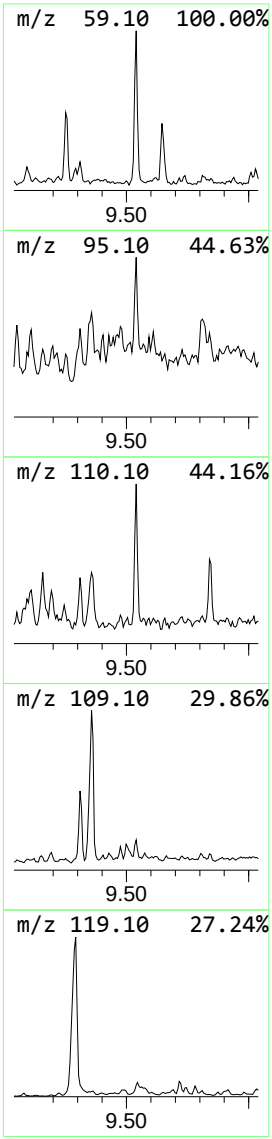
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 8-Hydroxycarvotanacetone Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.539	16.24 ng	502859	Acenaphthene-d10	9.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	8-Hydroxycarvotanacetone	168	C10H16O2	007712-46-1	53
2	S-(+)-5-(1-Hydroxy-1-methylethyl...	168	C10H16O2	060593-11-5	45
3	1-(4-Fluorophenyl)-2-methyl-2-pr...	168	C10H13FO	002928-17-8	37
4	5-Hydroxy-4-hydroxymethyl-1-(1-h...	186	C10H18O3	087096-72-8	25
5	4.beta.H,5.alpha.H-Eudesman-11-ol	224	C15H28O	031756-53-3	25





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Operator : CG\JU
Sample : N2154-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5

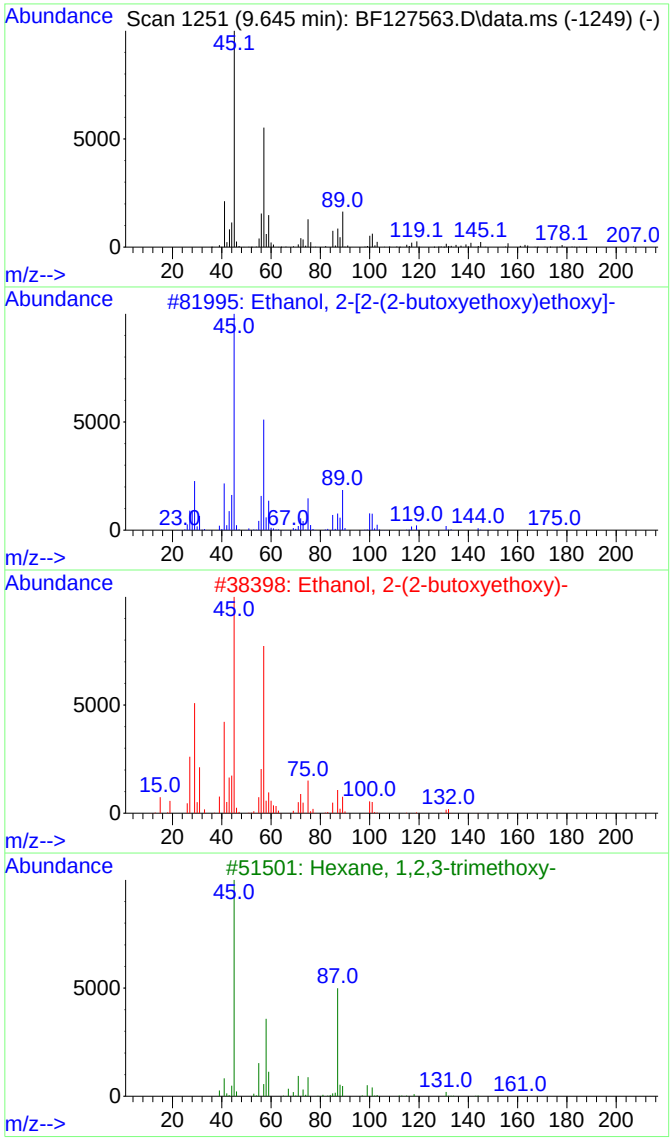
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

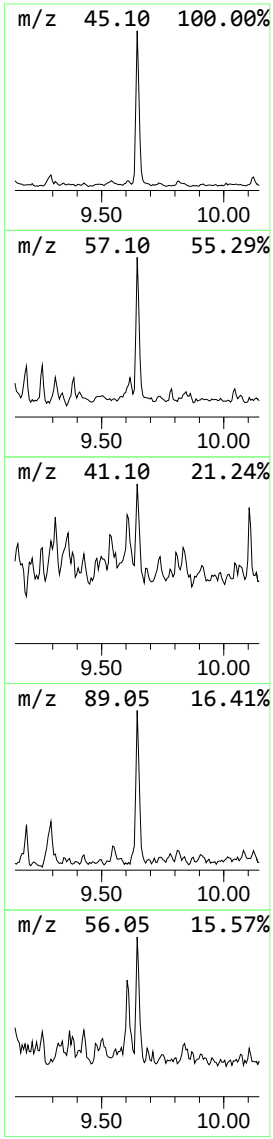
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 Ethanol, 2-[2-(2-butoxyetho... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.645	12.27 ng	379707	Acenaphthene-d10	9.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	91
2	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	78
3	Hexane, 1,2,3-trimethoxy-	176	C9H20O3	020637-29-0	72
4	Triethylene glycol	150	C6H14O4	000112-27-6	64
5	Ethanol, 2-[2-(ethenyloxy)ethoxy]-	132	C6H12O3	000929-37-3	59





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Sample : N2154-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
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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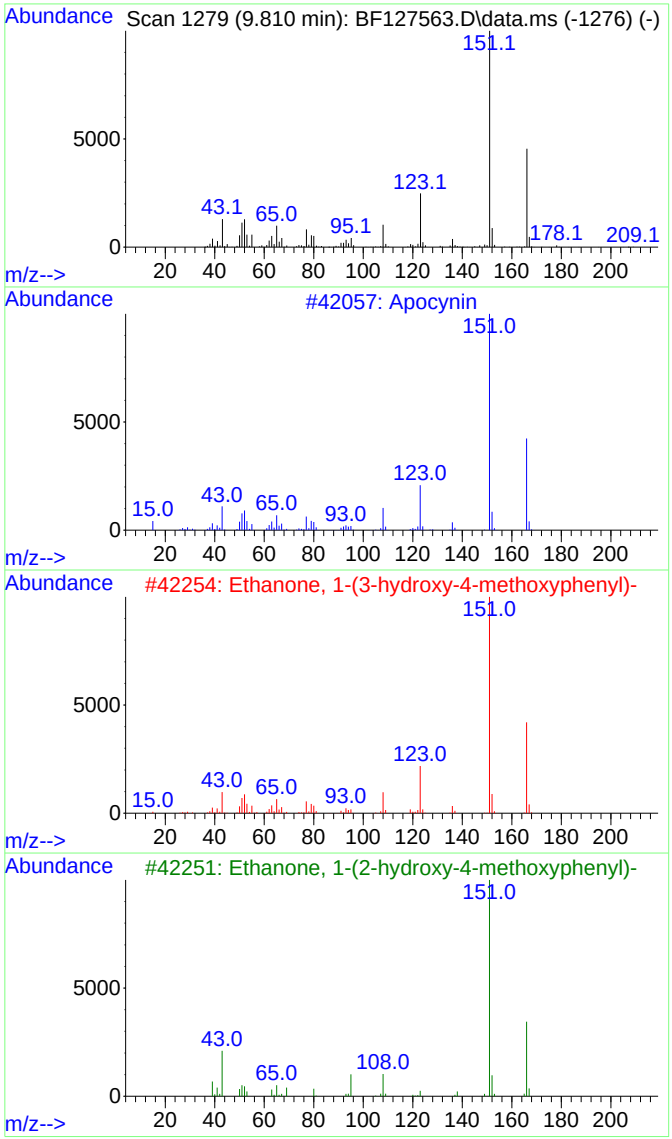
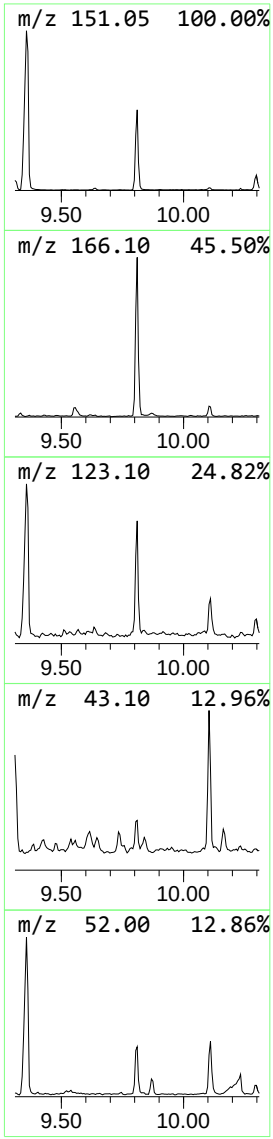
Peak Number 13 Apocynin Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.810	20.29 ng	628160	Acenaphthene-d10	9.875

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	94
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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Misc :
ALS Vial : 8 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

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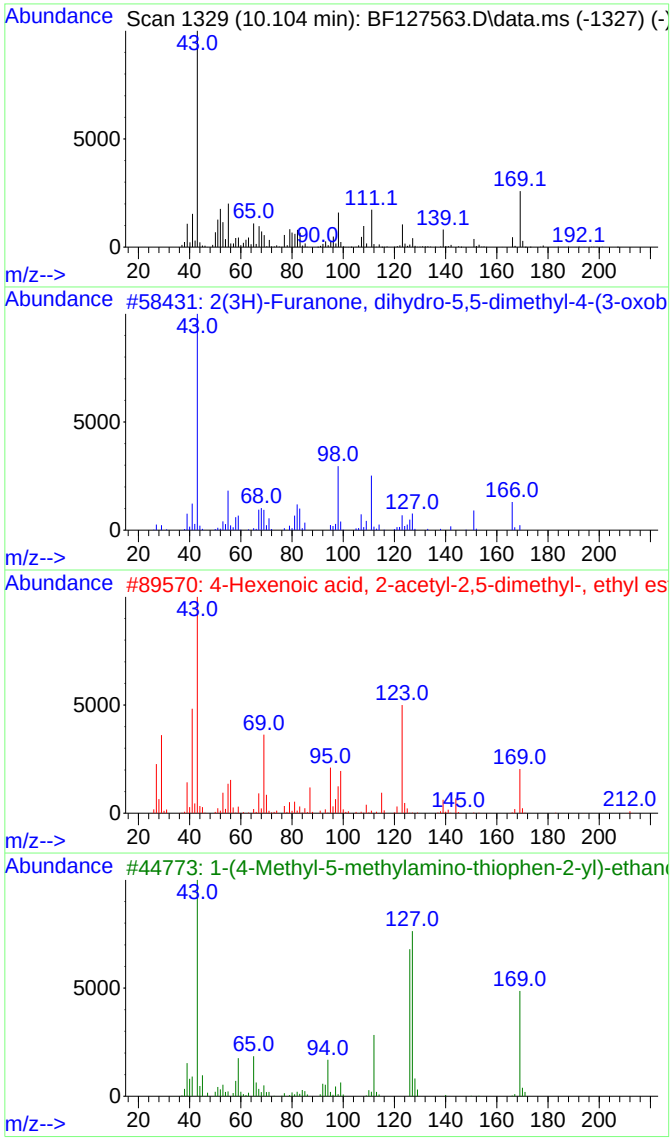
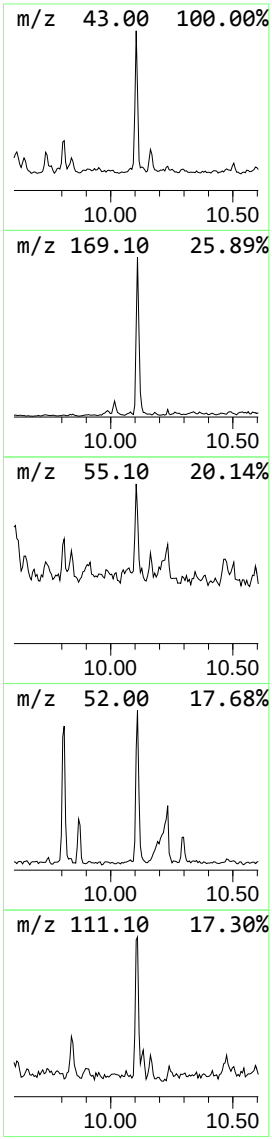
Peak Number 14 unknown10.104 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.104	19.38 ng	600051	Acenaphthene-d10	9.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Furanone, dihydro-5,5-dime...	184	C10H16O3	004436-81-1	22
2	4-Hexenoic acid, 2-acetyl-2,5-di...	212	C12H20O3	003132-71-6	17
3	1-(4-Methyl-5-methylamino-thioph...	169	C8H11NOS	1000275-72-3	9
4	6-methyl-1,2,3,4,5,6,7-[1,2,3]tr...	169	C3H3N7O2	1000444-20-2	9
5	Propanedioic acid, 2-propenyl-, ...	200	C10H16O4	002049-80-1	9





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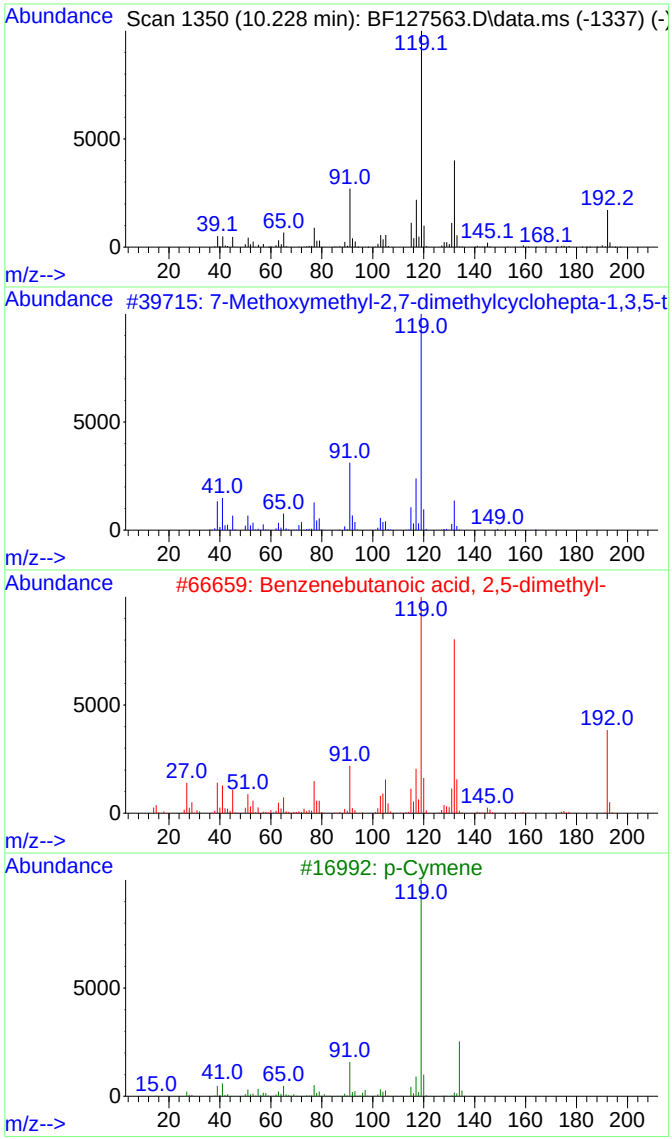
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

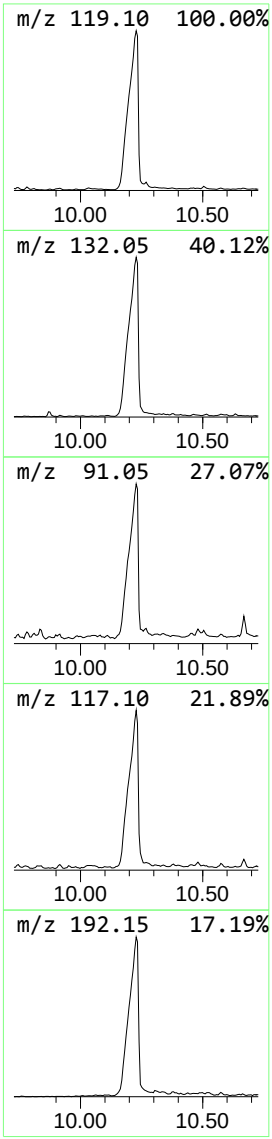
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 7-Methoxymethyl-2,7-dimethy... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.227	187.04 ng	5790340	Acenaphthene-d10	9.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Methoxymethyl-2,7-dimethylcycl...	164	C11H16O	073992-48-0	64
2	Benzenebutanoic acid, 2,5-dimethyl-	192	C12H16O2	001453-06-1	45
3	p-Cymene	134	C10H14	000099-87-6	43
4	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	43
5	o-Cymene	134	C10H14	000527-84-4	43





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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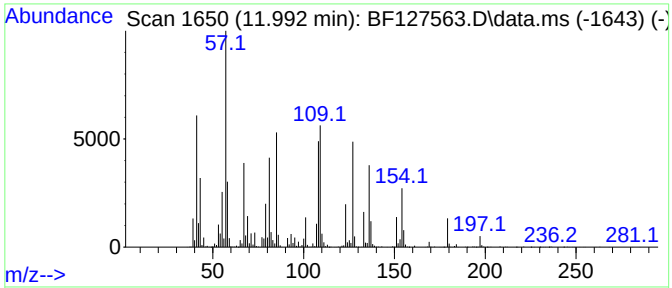
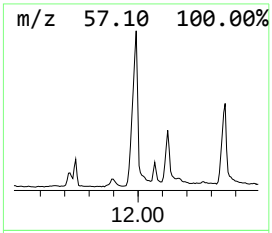
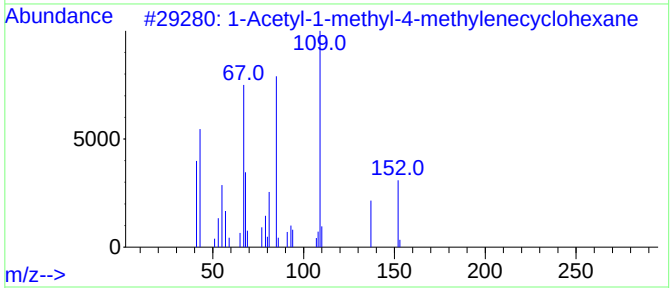
Peak Number 16 unknown11.992 Concentration Rank 2

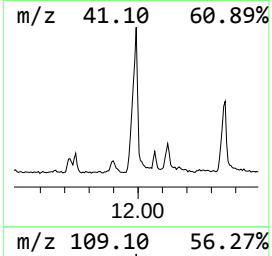
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.992	106.04 ng	2707200	Phenanthrene-d10	11.369

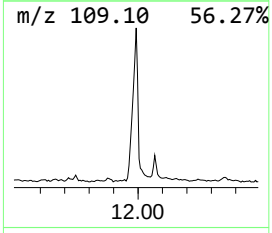
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Acetyl-1-methyl-4-methylenecyc...	152	C10H16O	1000424-28-4	38
2	2,5-Furandione, dihydro-3-(2-met...	154	C8H10O3	018908-20-8	35
3	1,4-Benzodioxin, 4a,5,6,7,8,8a-h...	154	C9H14O2	007196-96-5	22
4	3-Bromothiophenol, S-trimethylac...	272	C11H13BrOS	1000469-95-5	14
5	4-Nonanone, 2,6,8-trimethyl-	184	C12H24O	000123-18-2	11

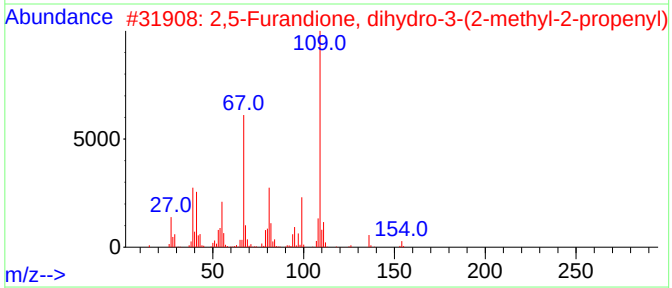


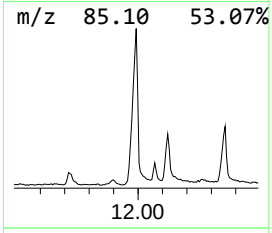


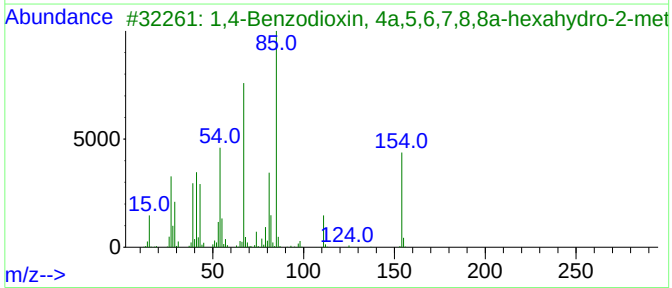


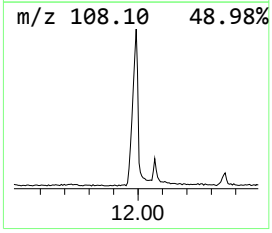












Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032922\
Data File : BF127563.D
Acq On : 29 Mar 2022 14:10
Operator : CG\JU
Sample : N2154-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

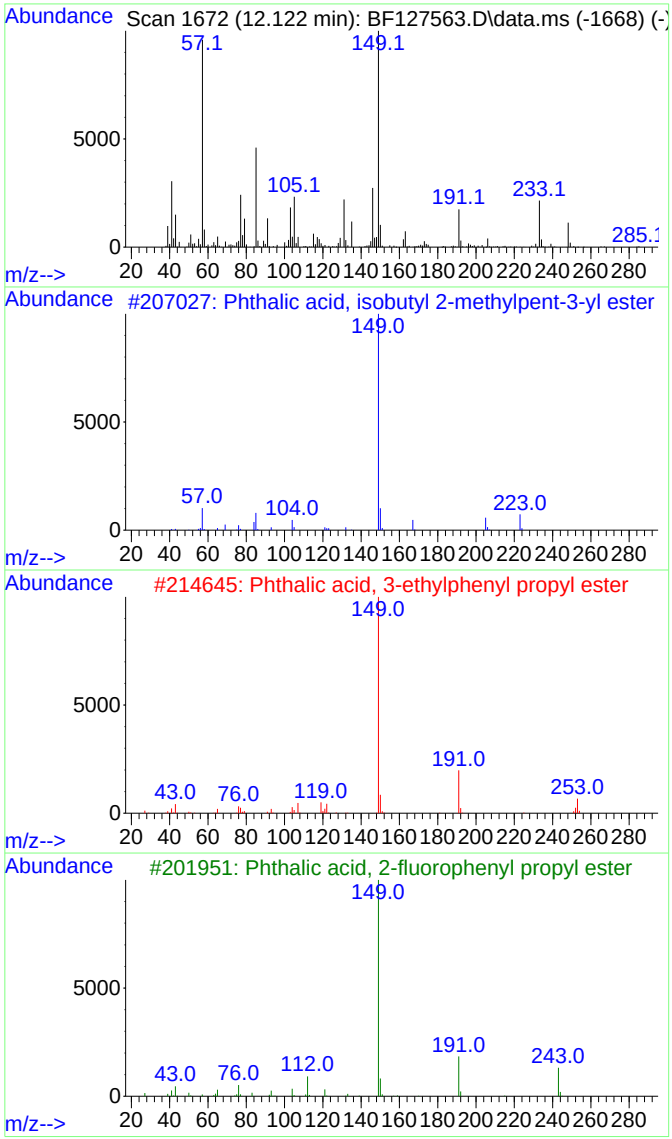
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

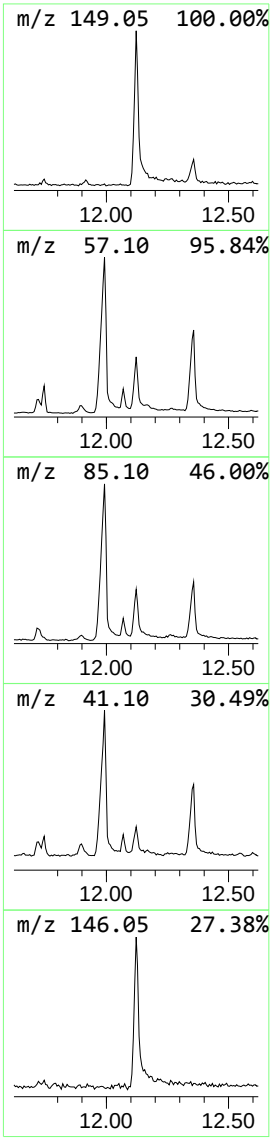
****

Peak Number 17 unknown12.121 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.121	21.78 ng	556129	Phenanthrene-d10	11.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic acid, isobutyl 2-methyl...	306	C18H26O4	1000356-90-7	47
2	Phthalic acid, 3-ethylphenyl pro...	312	C19H20O4	1000357-07-6	35
3	Phthalic acid, 2-fluorophenyl pr...	302	C17H15FO4	1000360-51-1	35
4	Phthalic acid, 5-methoxy-3-methy...	322	C18H26O5	1010314-88-4	35
5	Phthalic acid, 3,4-dimethylpheny...	354	C22H26O4	1000309-82-1	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032922\
Data File : BF127563.D
Acq On : 29 Mar 2022 14:10
Operator : CG\JU
Sample : N2154-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5

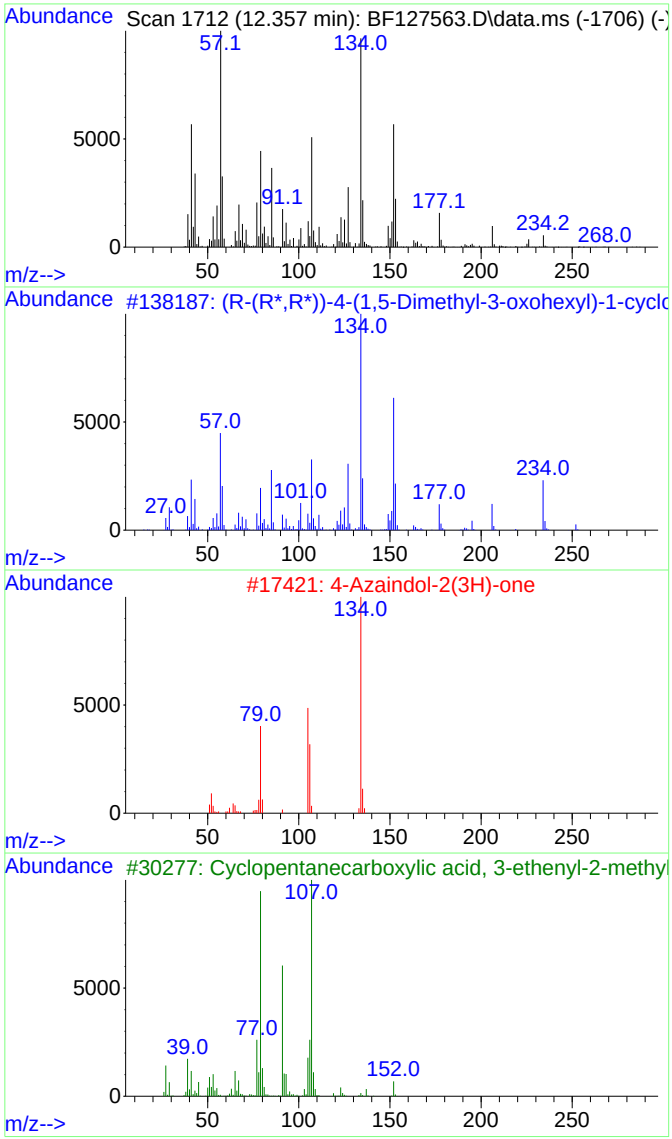
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

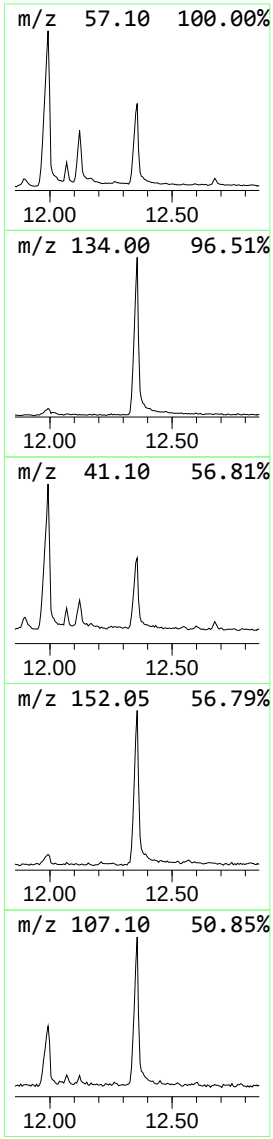
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 18 (R-(R*,R*))-4-(1,5-Dimethyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.357	58.46 ng	1492640	Phenanthrene-d10	11.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(R-(R*,R*))-4-(1,5-Dimethyl-3-ox...	252	C15H24O3	006753-22-6	78
2	4-Azaindol-2(3H)-one	134	C7H6N2O	032501-05-6	27
3	Cyclopentanecarboxylic acid, 3-e...	152	C9H12O2	108451-43-0	27
4	2-Amino-6-methylpyrimidine-4-car...	134	C6H6N4	064376-14-3	27
5	3-Hydroxy-4-methylbenzoic acid	152	C8H8O3	000586-30-1	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032922\
Data File : BF127563.D
Acq On : 29 Mar 2022 14:10
Operator : CG\JU
Sample : N2154-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5

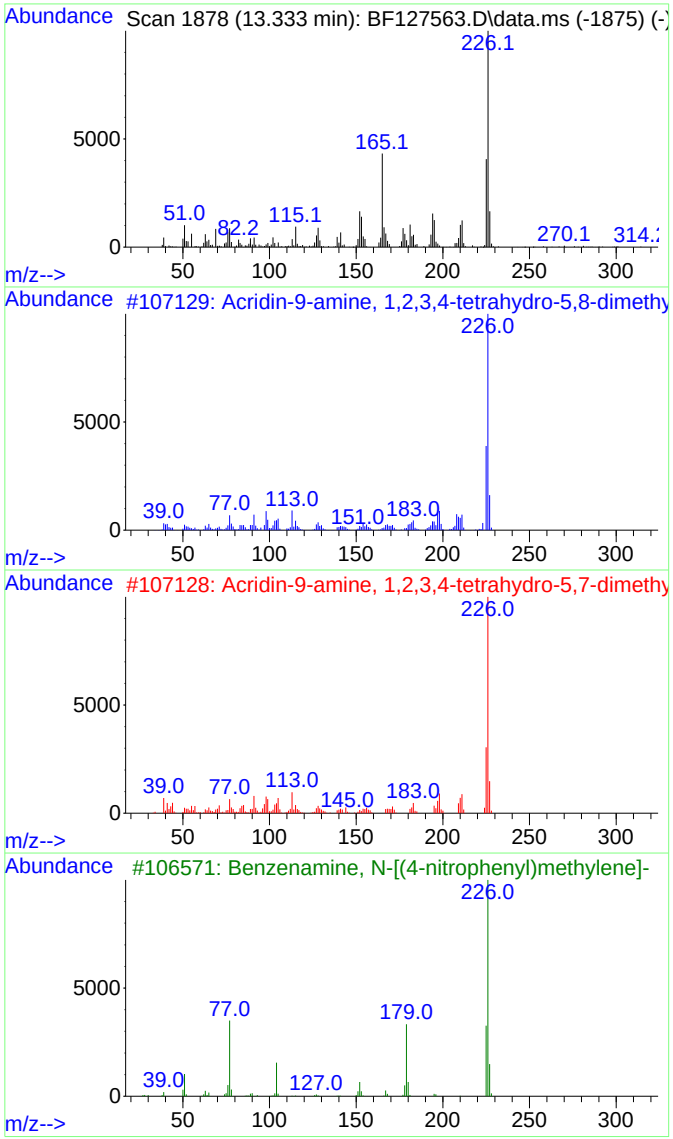
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

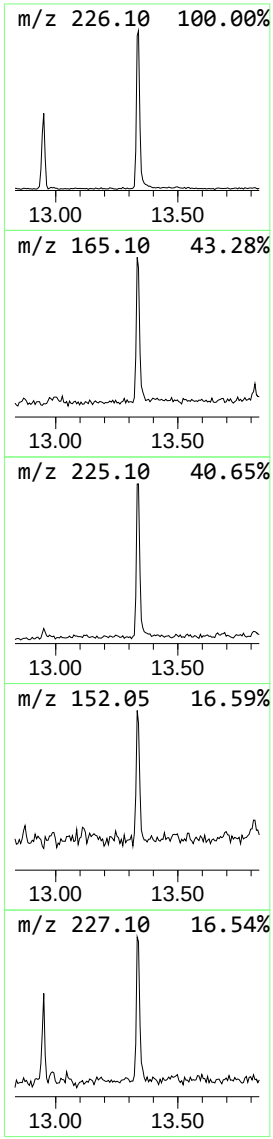
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 19 Acridin-9-amine, 1,2,3,4-te... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.333	18.84 ng	406434	Chrysene-d12	14.015

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acridin-9-amine, 1,2,3,4-tetrahy...	226	C15H18N2	297758-19-1	70
2	Acridin-9-amine, 1,2,3,4-tetrahy...	226	C15H18N2	1000300-57-6	58
3	Benzenamine, N-[(4-nitrophenyl)m...	226	C13H10N2O2	000785-80-8	55
4	9H-Pyrido[3,4-b]indole, 7-methox...	226	C14H14N2O	143502-37-8	52
5	4'-Methoxy-2-hydroxystilbene	226	C15H14O2	1000147-93-1	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032922\
Data File : BF127563.D
Acq On : 29 Mar 2022 14:10
Operator : CG\JU
Sample : N2154-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5

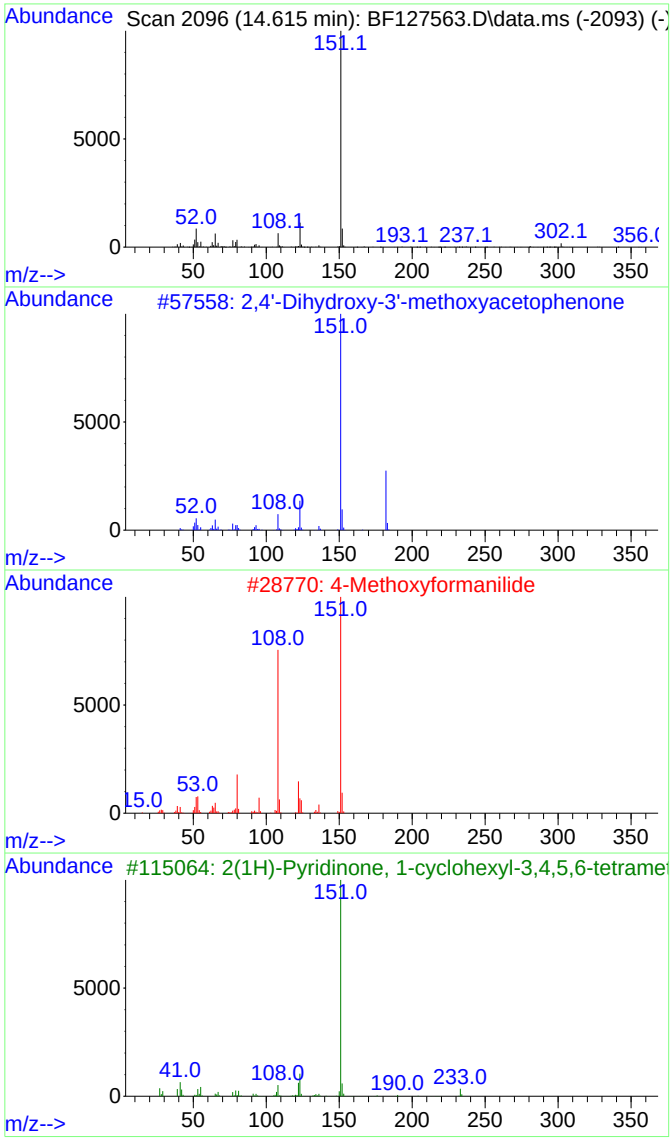
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

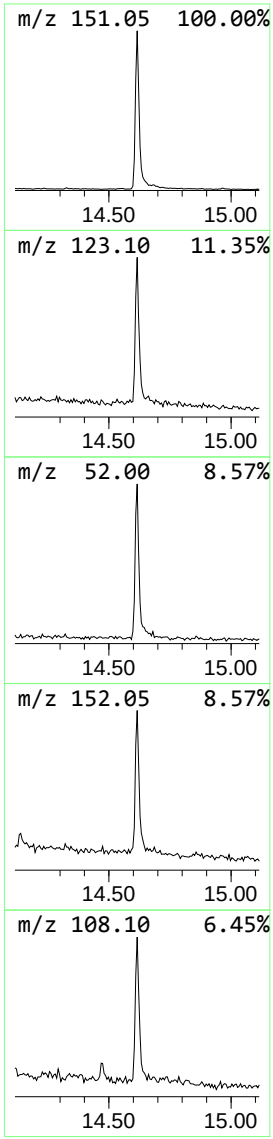
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 20 2,4'-Dihydroxy-3'-methoxyac... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.616	16.03 ng	345776	Chrysene-d12	14.015

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4'-Dihydroxy-3'-methoxyacetoph...	182	C9H10O4	018256-48-9	83
2	4-Methoxyformanilide	151	C8H9NO2	005470-34-8	72
3	2(1H)-Pyridinone, 1-cyclohexyl-3...	233	C15H23NO	082754-44-7	56
4	4'-Hydroxy-3'-methoxyacetophenon...	208	C12H16O3	1000395-32-8	56
5	1,4 Benzodioxan-6-amine	151	C8H9NO2	022013-33-8	45





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032922\
Data File : BF127563.D
Acq On : 29 Mar 2022 14:10
Operator : CG\JU
Sample : N2154-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.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
unknown6.898	6.898	12.7	ng	335502	1	6.834	527580	20.0
unknown7.281	7.281	16.5	ng	434692	1	6.834	527580	20.0
Bicyclo[2.2.1]h...	7.863	34.9	ng	1242610	2	8.116	711364	20.0
unknown7.922	7.922	12.2	ng	435417	2	8.116	711364	20.0
Bicyclo[2.2.1]h...	8.028	32.0	ng	1137060	2	8.116	711364	20.0
Bicyclo[3.1.1]h...	8.251	13.2	ng	467808	2	8.116	711364	20.0
exo-2-Hydroxyci...	8.357	15.9	ng	565766	2	8.116	711364	20.0
unknown8.916	8.916	12.8	ng	454281	2	8.116	711364	20.0
3,5-Dimethylphe...	9.292	22.9	ng	710210	3	9.875	619154	20.0
Vanillin	9.357	74.1	ng	2295250	3	9.875	619154	20.0
8-Hydroxycarvot...	9.539	16.2	ng	502859	3	9.875	619154	20.0
Ethanol, 2-[2-(...	9.645	12.3	ng	379707	3	9.875	619154	20.0
Apocynin	9.810	20.3	ng	628160	3	9.875	619154	20.0
unknown10.104	10.104	19.4	ng	600051	3	9.875	619154	20.0
7-Methoxymethyl...	10.227	187.0	ng	5790340	3	9.875	619154	20.0
unknown11.992	11.992	106.0	ng	2707200	4	11.369	510623	20.0
unknown12.121	12.121	21.8	ng	556129	4	11.369	510623	20.0
(R-(R*,R*))-4-(...	12.357	58.5	ng	1492640	4	11.369	510623	20.0
Acridin-9-amine...	13.333	18.8	ng	406434	5	14.015	431399	20.0
2,4'-Dihydroxy-...	14.616	16.0	ng	345776	5	14.015	431399	20.0