LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061221\
Data File : BF124290.D
Acq On : 12 Jun 2021 17:14
Operator : JU/CG
Sample : M2674-06 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TMR-DS-06-060921

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-BF060321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124290.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	6.398	729	733	738	rVV4	165815	271828	5.92%	0.342%
2	6.510	747	752	757	rVV3	418351	726444	15.83%	0.913%
3	6.663	775	778	786	rBV4	333002	590057	12.86%	0.742%
4	6.845	805	809	811	rBV	289182	272700	5.94%	0.343%
5	6.922	820	822	827	rVB4	199066	308576	6.72%	0.388%
6	7.016	833	838	843	rBV2	280641	447955	9.76%	0.563%
7	7.122	849	856	859	rVB2	879031	1080337	23.54%	1.358%
8	7.292	873	885	889	rBV2	1235603	2571524	56.03%	3.232%
9	7.357	894	896	898	rBV2	254541	235976	5.14%	0.297%
10	7.392	898	902	904	rBV	875674	837953	18.26%	1.053%
11	7.434	906	909	912	rVB3	207619	272510	5.94%	0.343%
12	7.492	916	919	922	rBV3	353172	297626	6.48%	0.374%
13	7.545	922	928	931	rBV3	597466	667700	14.55%	0.839%
14	7.575	931	933	936	rVB	497569	409316	8.92%	0.514%
15	7.628	936	942	947	rVB4	256188	503508	10.97%	0.633%
16	7.710	950	956	960	rBV	367198	437300	9.53%	0.550%
17	7.804	968	972	974	rBV3	871404	1246528	27.16%	1.567%
18	7.869	979	983	988	rVB5	234955	318463	6.94%	0.400%
19	7.945	988	996	999	rVB3	968020	1930575	42.06%	2.426%
20	8.010	1003	1007	1012	rVB2	661589	825340	17.98%	1.037%
21	8.069	1012	1017	1019	rBV5	358872	520774	11.35%	0.655%
22	8.104	1019	1023	1026	rBV	1818704	1634715	35.62%	2.055%
23	8.128	1026	1027	1029	rVV2	377604	296847	6.47%	0.373%
24	8.151	1029	1031	1034	rVB	477132	354404	7.72%	0.445%
25	8.204	1037	1040	1043	rVB3	353162	283583	6.18%	0.356%
26	8.233	1043	1045	1051	rVB2	307486	409052	8.91%	0.514%
27	8.304	1051	1057	1060	rBV	1083103	1159635	25.27%	1.458%
28	8.381	1067	1070	1073	rBV	607600	623027	13.57%	0.783%
29	8.410	1073	1075	1079	rVB2	317942	291641	6.35%	0.367%
30	8.510	1088	1092	1095	rBV	984008	1067043	23.25%	1.341%
31	8.563	1095	1101	1103	rBV4	433846	607041	13.23%	0.763%
32	8.610	1106	1109	1110	rVV	305980	241370	5.26%	0.303%
33	8.633	1110	1113	1117	rVB	1612113	1815852	39.56%	2.282%
34	8.716	1125	1127	1129	rBV2	466735	394319	8.59%	0.496%
35	8.745	1129	1132	1136	rVB3	405315	469424	10.23%	0.590%
36	8.786	1136	1139	1144	rVB3	335022	473176	10.31%	0.595%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061221\
Data File : BF124290.D
Acq On : 12 Jun 2021 17:14
Operator : JU/CG
Sample : M2674-06 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TMR-DS-06-060921

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-BF060321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	8.851	1146	1150	1151	rBV	855913	847690	18.47%	1.065%
38	8.880	1154	1155	1158	rVV2	364652	301127	6.56%	0.378%
39	8.916	1158	1161	1164	rVB3	532794	609123	13.27%	0.766%
40	8.945	1164	1166	1170	rVB3	556970	496348	10.81%	0.624%
41	9.075	1177	1188	1190	rBV	2962370	4581697	99.82%	5.759%
42	9.098	1190	1192	1195	rVV3	508502	413539	9.01%	0.520%
43	9.151	1198	1201	1204	rVB2	1397053	1387456	30.23%	1.744%
44	9.210	1208	1211	1214	rVB3	408160	464006	10.11%	0.583%
45	9.263	1214	1220	1221	rBV5	541558	918976	20.02%	1.155%
46	9.286	1221	1224	1226	rVB3	463780	466341	10.16%	0.586%
47	9.410	1243	1245	1248	rVB2	305582	292281	6.37%	0.367%
48	9.480	1252	1257	1262	rBV5	595913	1164419	25.37%	1.464%
49	9.586	1266	1275	1277	rBV3	3116029	4589737	100.00%	5.769%
50	9.628	1279	1282	1284	rVB	1000852	711846	15.51%	0.895%
51	9.816	1311	1314	1316	rBV2	441825	499814	10.89%	0.628%
52	9.845	1316	1319	1321	rVV2	477194	530606	11.56%	0.667%
53	9.892	1325	1327	1330	rBV2	326622	282940	6.16%	0.356%
54	9.980	1335	1342	1345	rBV	3164657	4289238	93.45%	5.391%
55	10.045	1350	1353	1355	rVB	477064	417180	9.09%	0.524%
56	10.080	1355	1359	1361	rBV4	597213	837735	18.25%	1.053%
57	10.239	1383	1386	1390	rVB4	234768	326752	7.12%	0.411%
58	10.280	1390	1393	1395	rBV2	318115	361778	7.88%	0.455%
59	10.310	1396	1398	1402	rVV3	494485	554284	12.08%	0.697%
60	10.351	1402	1405	1408	rVV	457536	498114	10.85%	0.626%
61	10.392	1408	1412	1415	rVV	2705168	2823503	61.52%	3.549%
62	10.439	1417	1420	1422	rVB2	311711	317791	6.92%	0.399%
63	10.592	1443	1446	1450	rVB4	342994	384157	8.37%	0.483%
64	10.674	1457	1460	1466	rVB3	749955	938571	20.45%	1.180%
65	10.727	1466	1469	1472	rBV3	158274	242681	5.29%	0.305%
66	10.845	1484	1489	1492	rBV2	899124	1037195	22.60%	1.304%
67	10.910	1498	1500	1503	rVB3	299101	251389	5.48%	0.316%
68	10.951	1503	1507	1510	rBV5	152593	237596	5.18%	0.299%
69	11.016	1510	1518	1520	rBV2	1255345	2093938	45.62%	2.632%
70	11.157	1537	1542	1545	rVB	982533	1064501	23.19%	1.338%
71	11.233	1552	1555	1557	rBV2	386494	318646	6.94%	0.400%
72	11.404	1582	1584	1587	rVB	750794	718854	15.66%	0.904%
73	11.492	1596	1599	1604	rBV7	242407	276554	6.03%	0.348%
74	11.663	1625	1628	1631	rBV	309986	299652	6.53%	0.377%
75	11.769	1643	1646	1650	rVB5	216265	242278	5.28%	0.305%
76	11.921	1668	1672	1675	rVB2	820174	895529	19.51%	1.126%

LSC Area Percent Report

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Acq On : 12 Jun 2021 17:14
Operator : JU/CG
Sample : M2674-06 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TMR-DS-06-060921

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-BF060321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	12.439	1755	1760	1761	rBV3	301577	419264	9.13%	0.527%
78	12.457	1761	1763	1767	rVV	513058	451941	9.85%	0.568%
79	12.627	1785	1792	1794	rBV4	422519	834718	18.19%	1.049%
80	12.816	1821	1824	1825	rBV	829757	681217	14.84%	0.856%
81	12.833	1825	1827	1832	rVB	703002	609163	13.27%	0.766%
82	13.445	1929	1931	1936	rVB	338552	332346	7.24%	0.418%
83	13.515	1940	1943	1950	rVB3	784459	1044381	22.75%	1.313%
84	13.863	1998	2002	2008	rVB	1950161	1960304	42.71%	2.464%
85	13.957	2015	2018	2021	rVB	536851	452389	9.86%	0.569%
86	14.033	2028	2031	2034	rVB	277147	264473	5.76%	0.332%
87	14.092	2036	2041	2044	rVV3	1013049	1280423	27.90%	1.609%
88	14.121	2044	2046	2051	rVV2	397623	394582	8.60%	0.496%
89	14.174	2051	2055	2058	rVV2	463521	756405	16.48%	0.951%
90	14.204	2058	2060	2063	rVB	543668	422270	9.20%	0.531%
91	14.498	2106	2110	2115	rVB2	1658914	1668913	36.36%	2.098%
92	14.574	2120	2123	2126	rVB	447162	435425	9.49%	0.547%
93	14.710	2142	2146	2150	rBV3	626785	910633	19.84%	1.145%
94	14.821	2162	2165	2167	rBV2	290649	326192	7.11%	0.410%
95	15.168	2221	2224	2231	rVB2	183242	252143	5.49%	0.317%
96	15.757	2321	2324	2328	rVB2	302692	391115	8.52%	0.492%
97	15.927	2349	2353	2358	rVB6	236514	363640	7.92%	0.457%
98	16.009	2361	2367	2371	rVV	554038	873694	19.04%	1.098%
99	16.233	2398	2405	2412	rVB6	560695	1262718	27.51%	1.587%
100	18.133	2722	2728	2735	rVB6	121231	294833	6.42%	0.371%

Sum of corrected areas: 79563163

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061221\
Data File : BF124290.D
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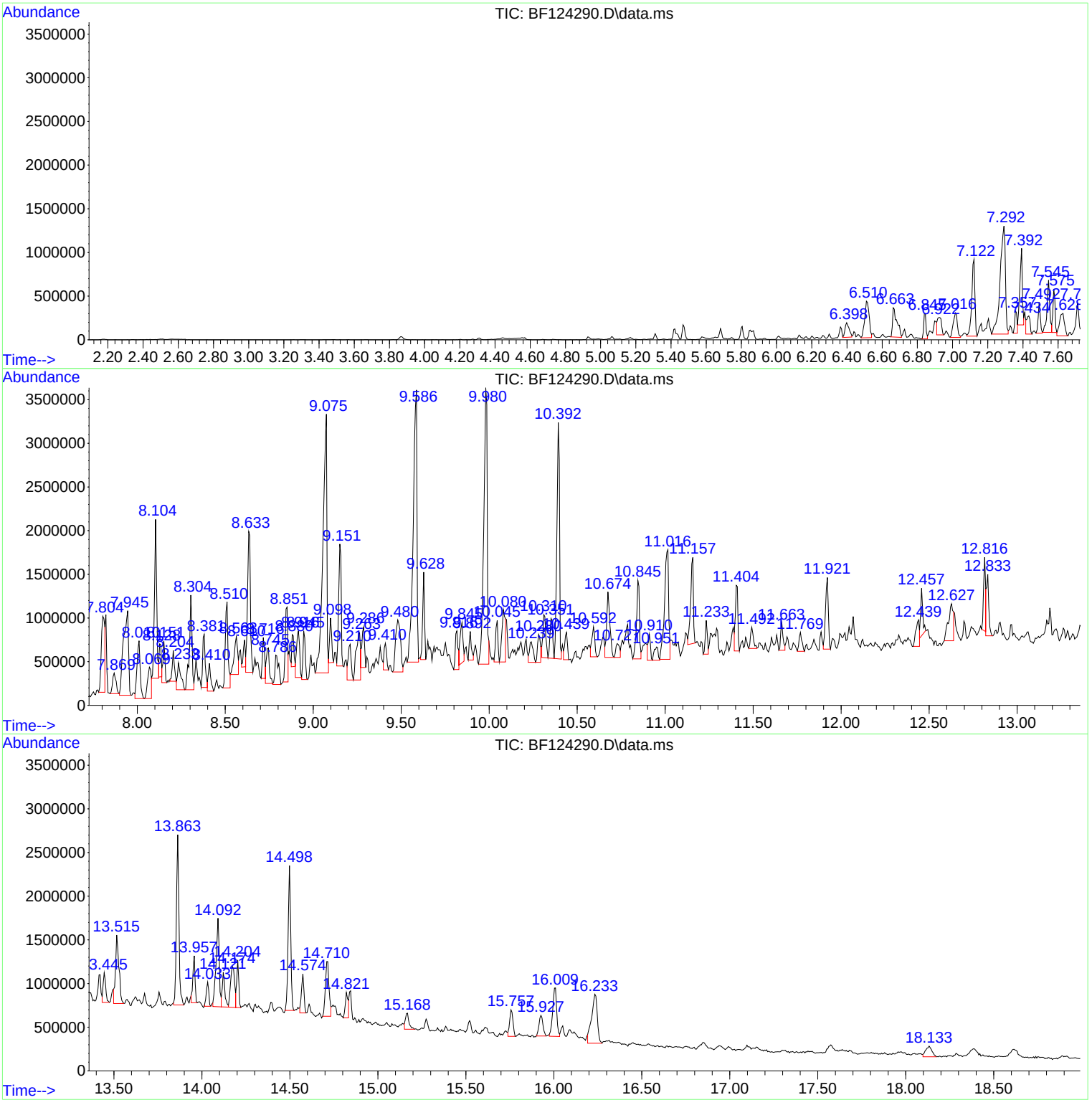
Sample : M2674-06 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TMR-DS-06-060921

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061221\
Data File : BF124290.D
Acq On : 12 Jun 2021 17:14
Operator : JU/CG
Sample : M2674-06 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TMR-DS-06-060921

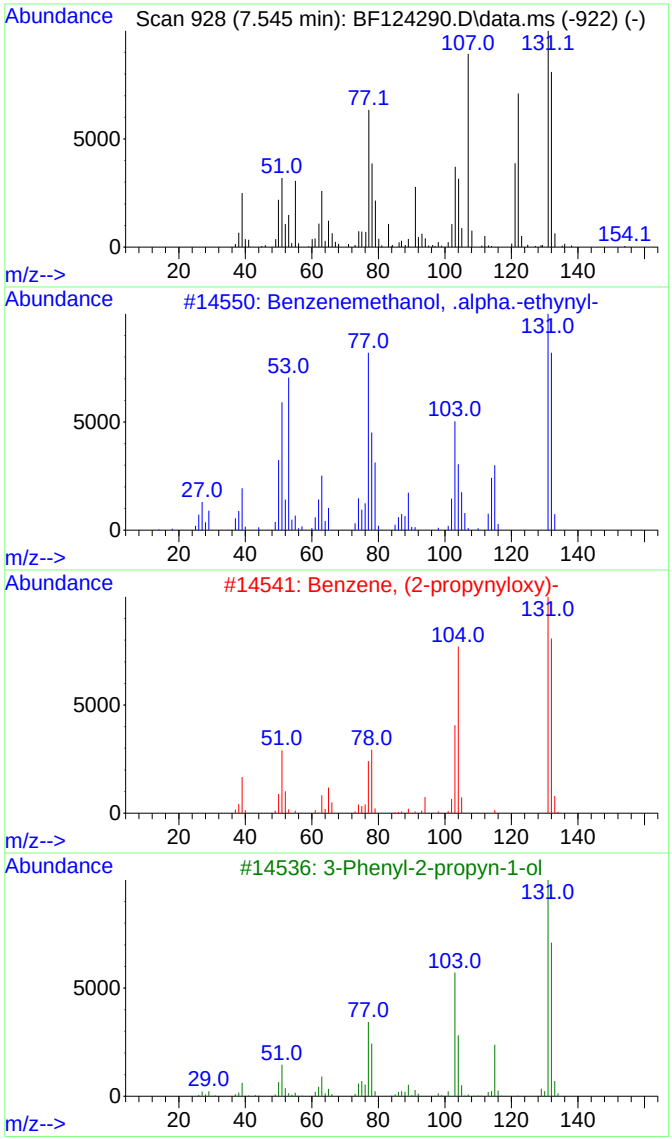
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

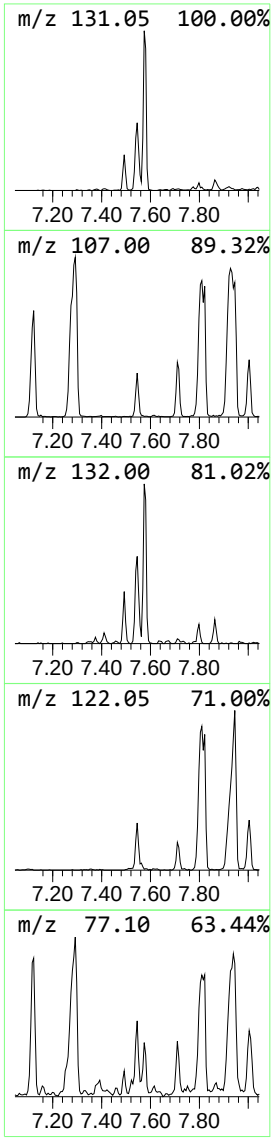
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Benzenemethanol, .alpha.-et... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.545	44.99 ng	667700	Naphthalene-d8	8.128

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenemethanol, .alpha.-ethynyl-	132	C9H8O	004187-87-5	70
2	Benzene, (2-propynyloxy)-	132	C9H8O	013610-02-1	60
3	3-Phenyl-2-propyn-1-ol	132	C9H8O	001504-58-1	52
4	2-Propenal, 3-phenyl-	132	C9H8O	000104-55-2	50
5	Phenol, 2,4-dimethyl-	122	C8H10O	000105-67-9	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061221\
Data File : BF124290.D
Acq On : 12 Jun 2021 17:14
Operator : JU/CG
Sample : M2674-06 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TMR-DS-06-060921

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

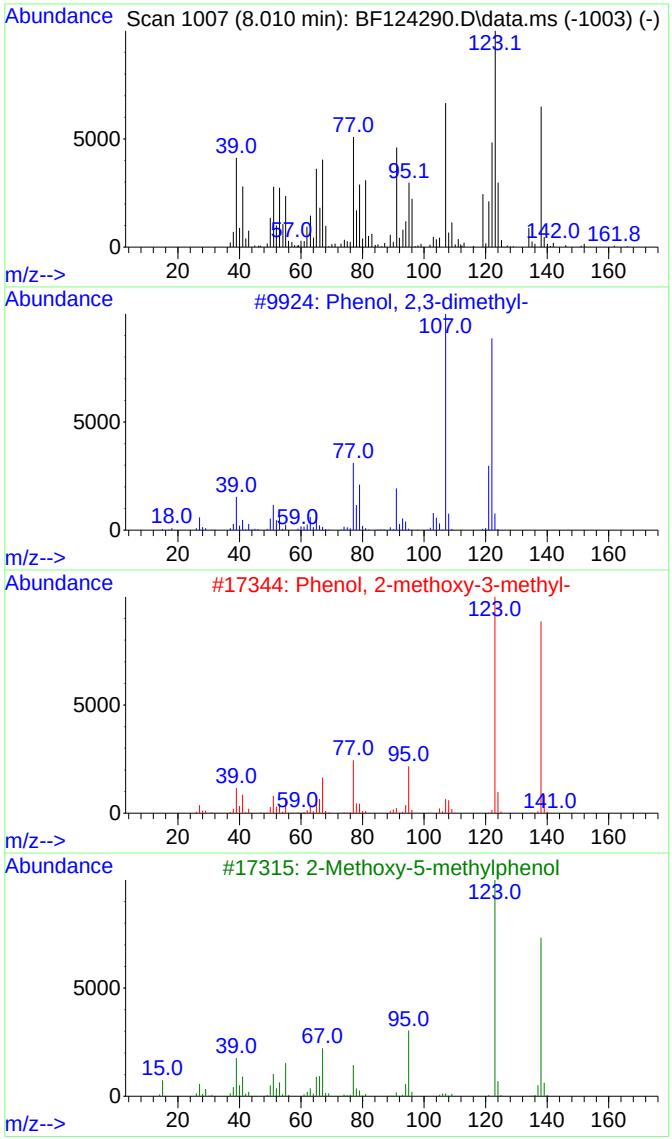
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

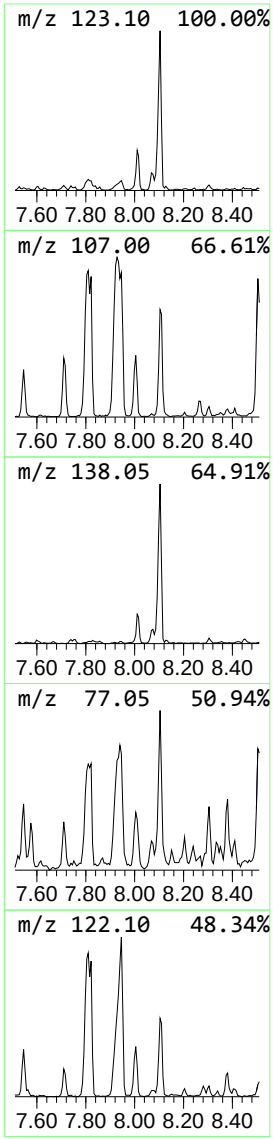
****

Peak Number 2 Phenol, 2,3-dimethyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.010	55.61 ng	825340	Naphthalene-d8	8.128

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,3-dimethyl-	122	C8H10O	000526-75-0	72
2	Phenol, 2-methoxy-3-methyl-	138	C8H10O2	018102-31-3	49
3	2-Methoxy-5-methylphenol	138	C8H10O2	001195-09-1	41
4	Phenol, 3,5-dimethyl-	122	C8H10O	000108-68-9	38
5	Phenol, 2,5-dimethyl-	122	C8H10O	000095-87-4	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061221\
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Instrument :
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ClientSampleId :
TMR-DS-06-060921

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

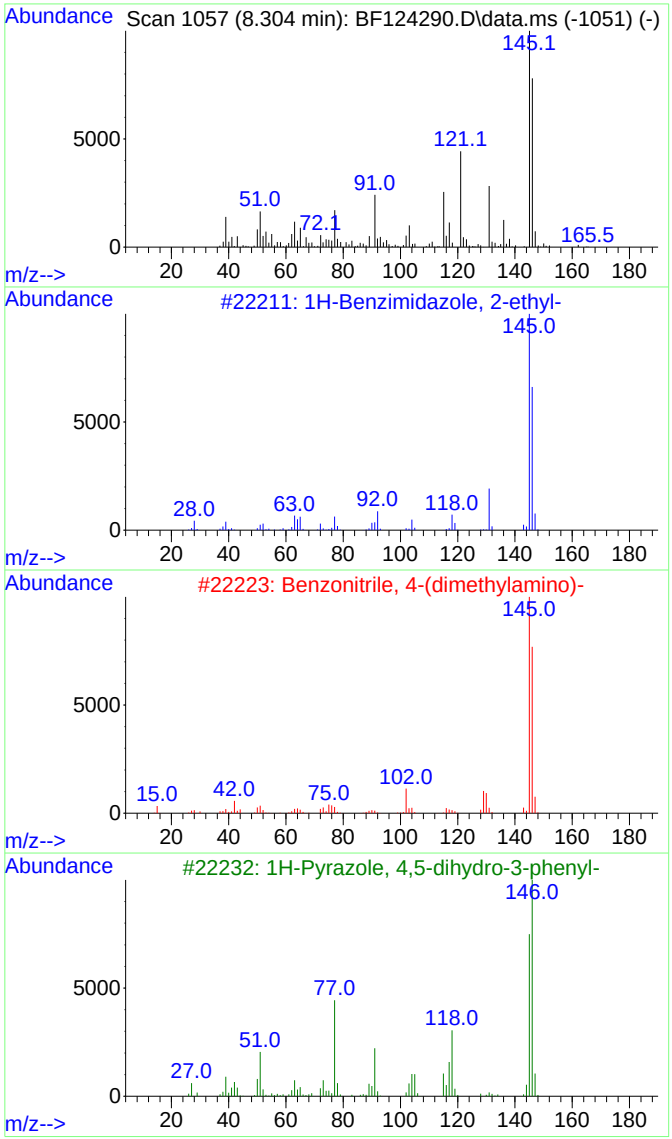
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

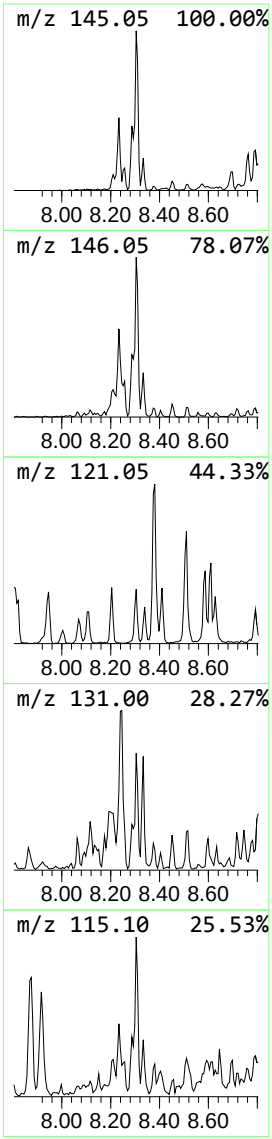
****

Peak Number 3 1H-Benzimidazole, 2-ethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.304	78.13 ng	1159640	Naphthalene-d8	8.128

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzimidazole, 2-ethyl-	146	C9H10N2	001848-84-6	53
2	Benzonitrile, 4-(dimethylamino)-	146	C9H10N2	001197-19-9	50
3	1H-Pyrazole, 4,5-dihydro-3-phenyl-	146	C9H10N2	000936-48-1	43
4	1,2-Dimethylbenzimidazole	146	C9H10N2	002876-08-6	43
5	1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061221\
Data File : BF124290.D
Acq On : 12 Jun 2021 17:14
Operator : JU/CG
Sample : M2674-06 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TMR-DS-06-060921

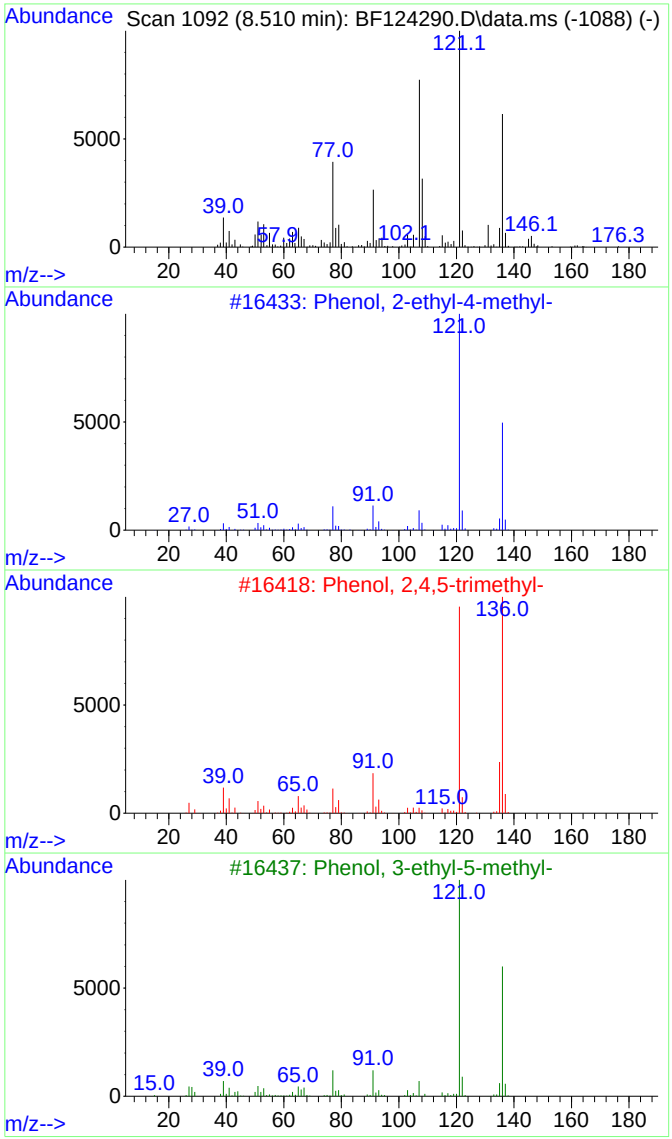
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

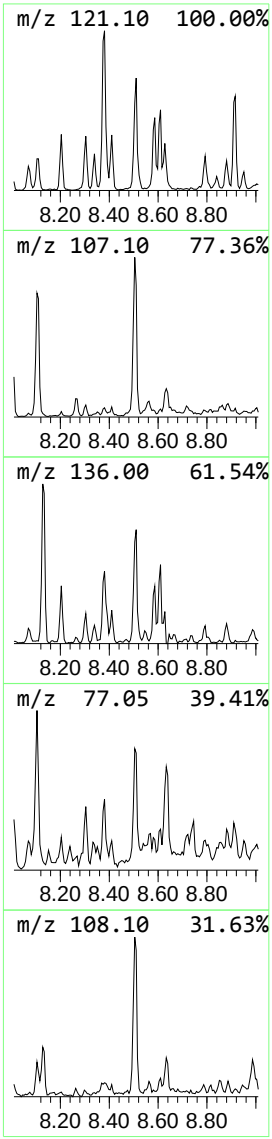
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Phenol, 2-ethyl-4-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.510	71.89 ng	1067040	Naphthalene-d8	8.128

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-ethyl-4-methyl-	136	C9H12O	003855-26-3	60
2	Phenol, 2,4,5-trimethyl-	136	C9H12O	000496-78-6	49
3	Phenol, 3-ethyl-5-methyl-	136	C9H12O	000698-71-5	49
4	Phenol, 3-(1-methylethyl)-	136	C9H12O	000618-45-1	46
5	Benzene, 1-ethyl-4-methoxy-	136	C9H12O	001515-95-3	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061221\
Data File : BF124290.D
Acq On : 12 Jun 2021 17:14
Operator : JU/CG
Sample : M2674-06 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TMR-DS-06-060921

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

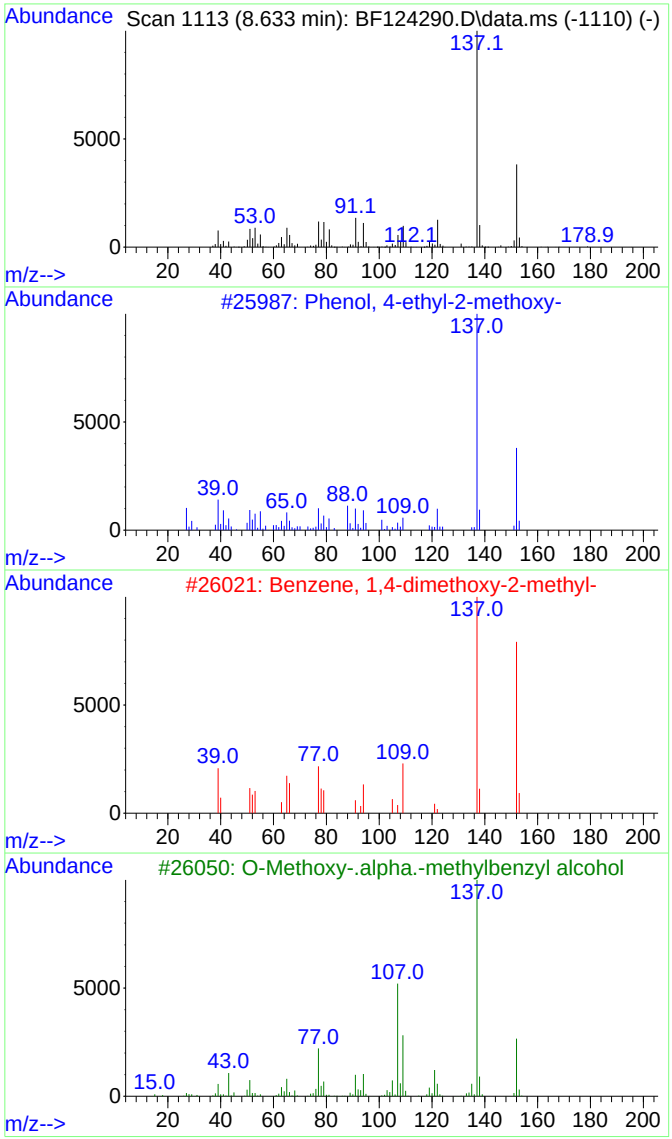
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

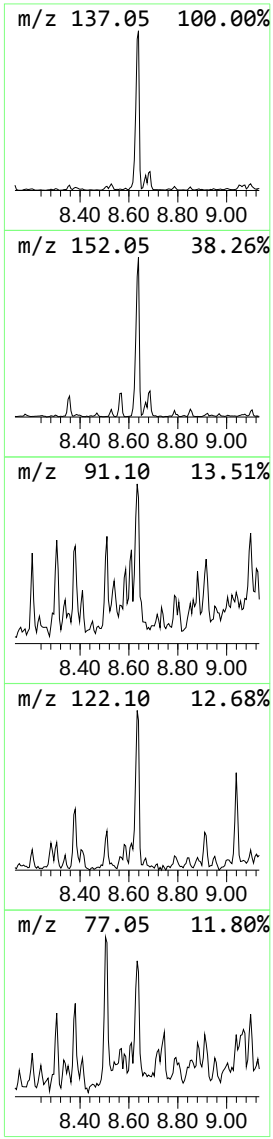
****

Peak Number 5 Phenol, 4-ethyl-2-methoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.633	122.34 ng	1815850	Naphthalene-d8	8.128

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-ethyl-2-methoxy-	152	C9H12O2	002785-89-9	95
2	Benzene, 1,4-dimethoxy-2-methyl-	152	C9H12O2	024599-58-4	83
3	O-Methoxy-.alpha.-methylbenzyl a...	152	C9H12O2	013513-82-1	80
4	4-Isopropylthiophenol	152	C9H12S	004946-14-9	72
5	Resorcinol, 2-acetyl-	152	C8H8O3	000699-83-2	64





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Acq On : 12 Jun 2021 17:14
Operator : JU/CG
Sample : M2674-06 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TMR-DS-06-060921

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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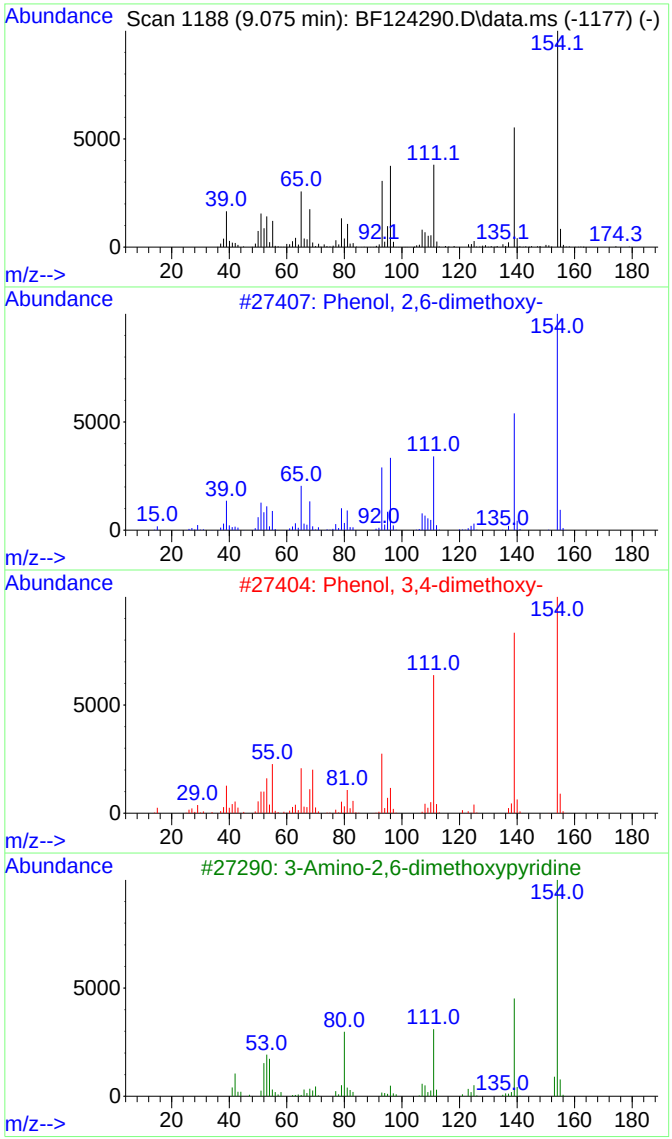
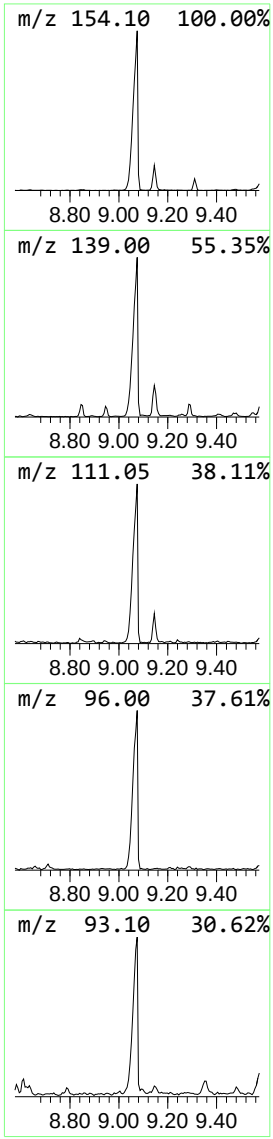
Peak Number 6 Phenol, 2,6-dimethoxy- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.075	323.86 ng	4581700	Acenaphthene-d10	9.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,6-dimethoxy-	154	C8H10O3	000091-10-1	98
2	Phenol, 3,4-dimethoxy-	154	C8H10O3	002033-89-8	83
3	3-Amino-2,6-dimethoxypyridine	154	C7H10N2O2	028020-37-3	53
4	2-Thiophenecarboxamide, N-[2-(2-...	291	C15H17NO3S	1000337-61-7	38
5	5-Fluoro-2-hydroxyacetophenone	154	C8H7FO2	000394-32-1	38





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Operator : JU/CG
Sample : M2674-06 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TMR-DS-06-060921

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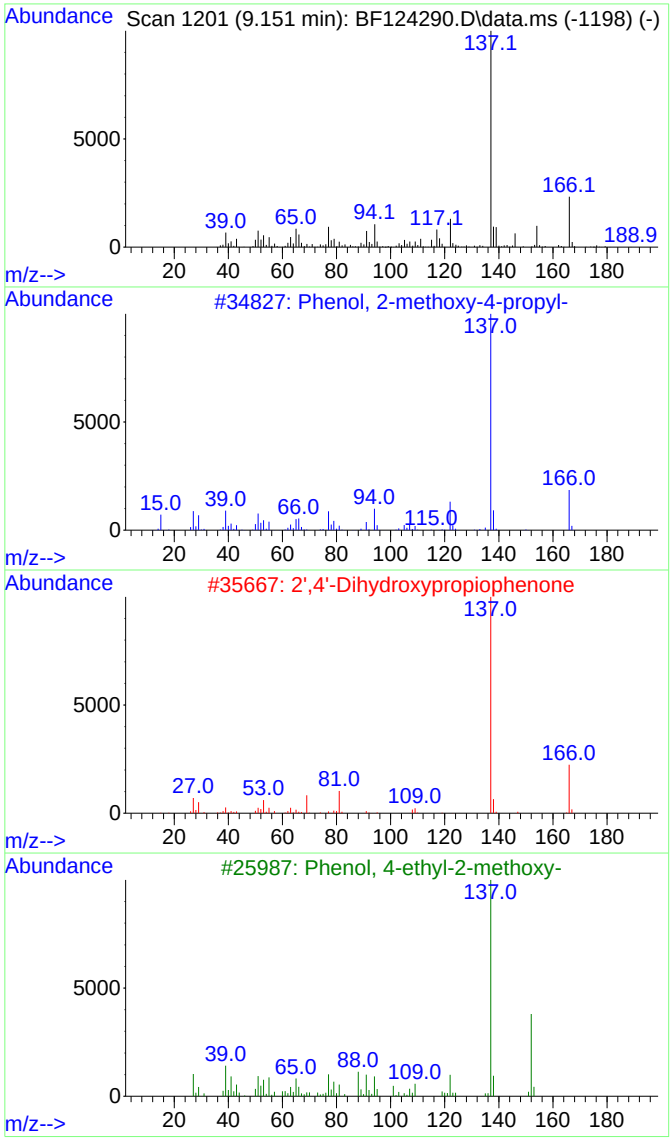
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

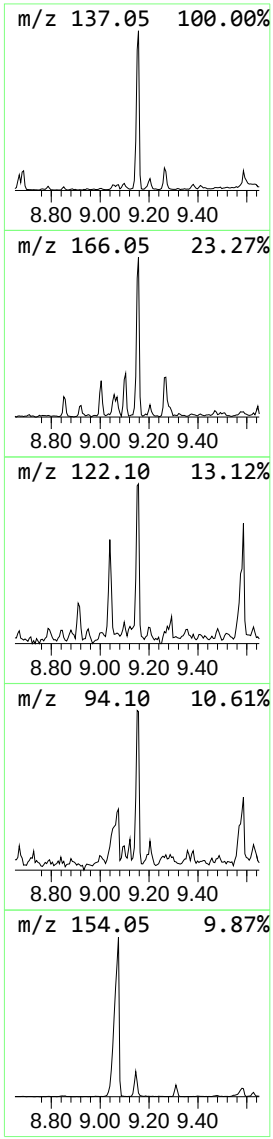
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Phenol, 2-methoxy-4-propyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.151	98.07 ng	1387460	Acenaphthene-d10	9.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-methoxy-4-propyl-	166	C10H14O2	002785-87-7	93
2	2',4'-Dihydroxypropiophenone	166	C9H10O3	005792-36-9	52
3	Phenol, 4-ethyl-2-methoxy-	152	C9H12O2	002785-89-9	50
4	Ethyl Vanillin	166	C9H10O3	000121-32-4	49
5	Phenol, 3-(dimethylamino)-	137	C8H11NO	000099-07-0	47





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Sample : M2674-06 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TMR-DS-06-060921

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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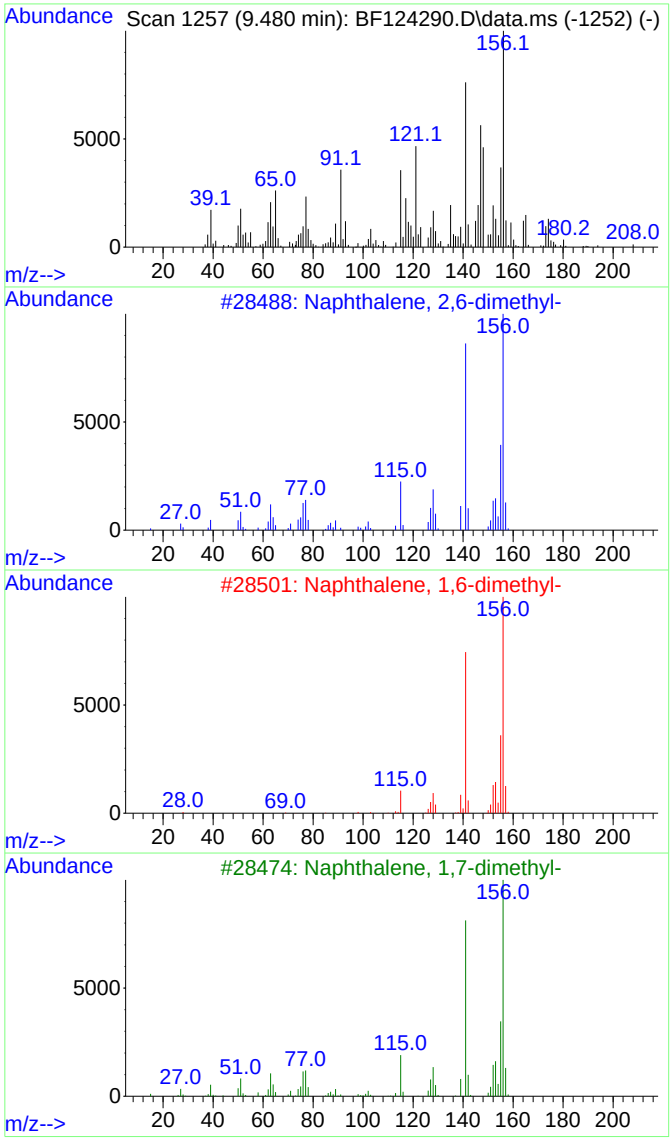
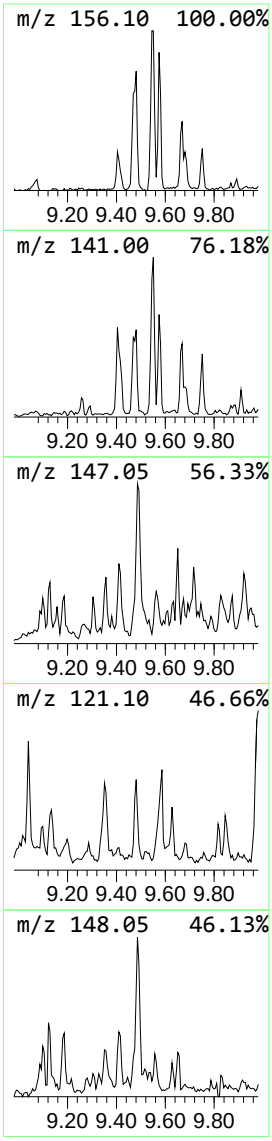
Peak Number 8 Naphthalene, 2,6-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.480	82.31 ng	1164420	Acenaphthene-d10	9.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	94
2	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	90
3	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	89
4	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	89
5	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	87





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Operator : JU/CG
Sample : M2674-06 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TMR-DS-06-060921

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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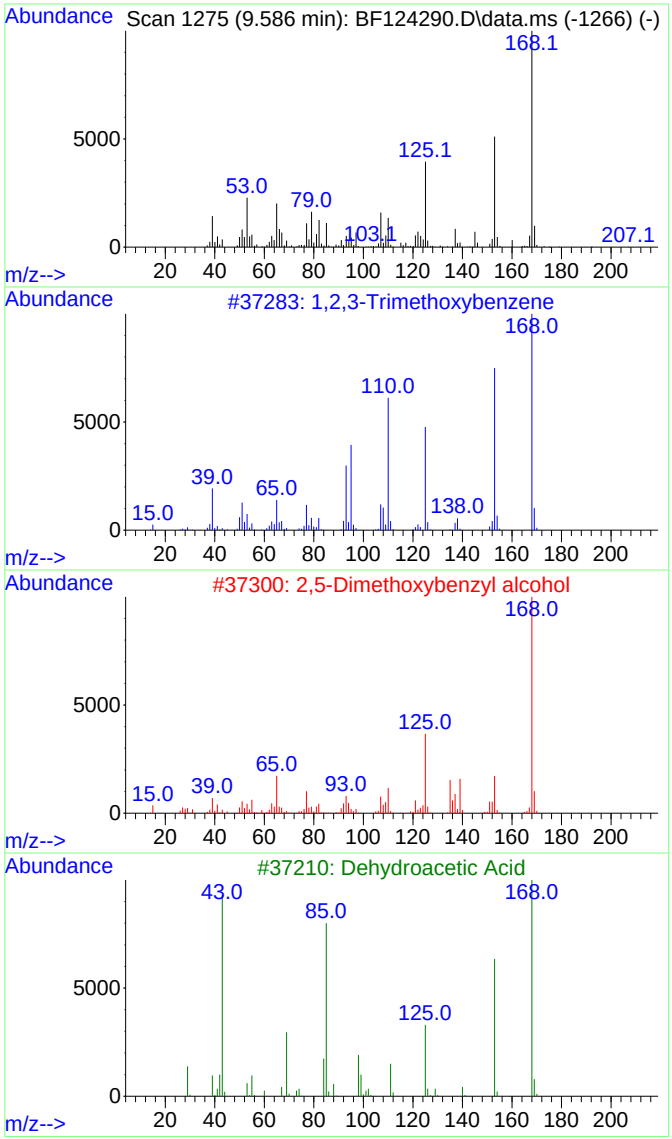
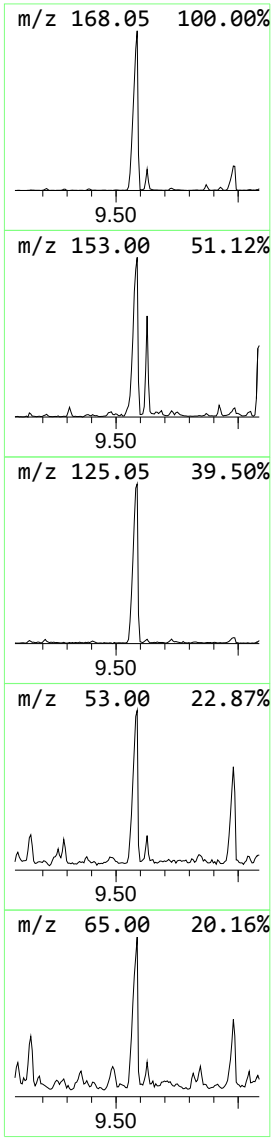
Peak Number 9 1,2,3-Trimethoxybenzene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.586	324.43 ng	4589740	Acenaphthene-d10	9.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,3-Trimethoxybenzene	168	C9H12O3	000634-36-6	76
2	2,5-Dimethoxybenzyl alcohol	168	C9H12O3	033524-31-1	60
3	Dehydroacetic Acid	168	C8H8O4	000520-45-6	53
4	3-Hydroxy-4-methoxybenzoic acid	168	C8H8O4	000645-08-9	49
5	Benzoic acid, 4-hydroxy-3-methoxy-	168	C8H8O4	000121-34-6	46





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Operator : JU/CG
Sample : M2674-06 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TMR-DS-06-060921

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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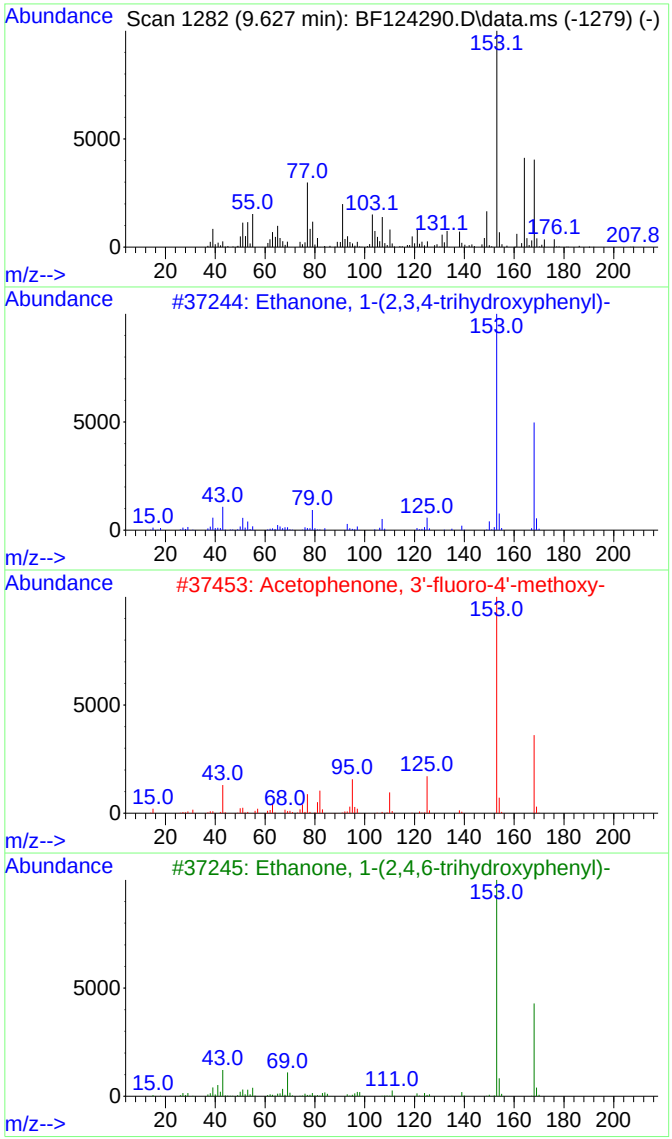
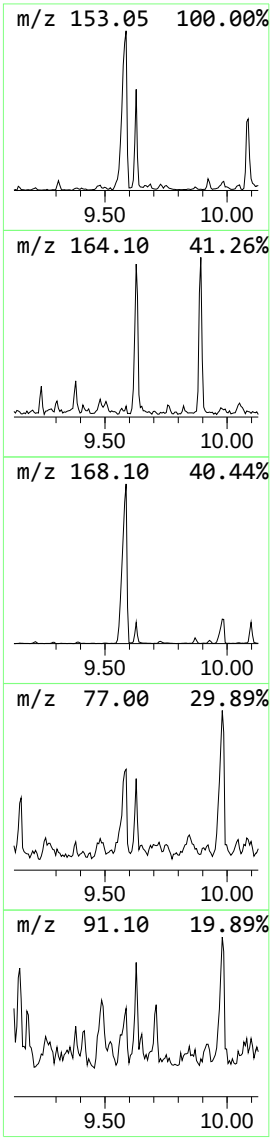
Peak Number 10 unknown9.627 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.627	50.32 ng	711846	Acenaphthene-d10	9.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanone, 1-(2,3,4-trihydroxyphe...	168	C8H8O4	000528-21-2	46
2	Acetophenone, 3'-fluoro-4'-methoxy-	168	C9H9FO2	000455-91-4	46
3	Ethanone, 1-(2,4,6-trihydroxyphe...	168	C8H8O4	000480-66-0	43
4	2-Methyl-5-nitrophenol	153	C7H7NO3	005428-54-6	41
5	5-Methyl-2-nitrophenol	153	C7H7NO3	000700-38-9	38





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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TMR-DS-06-060921

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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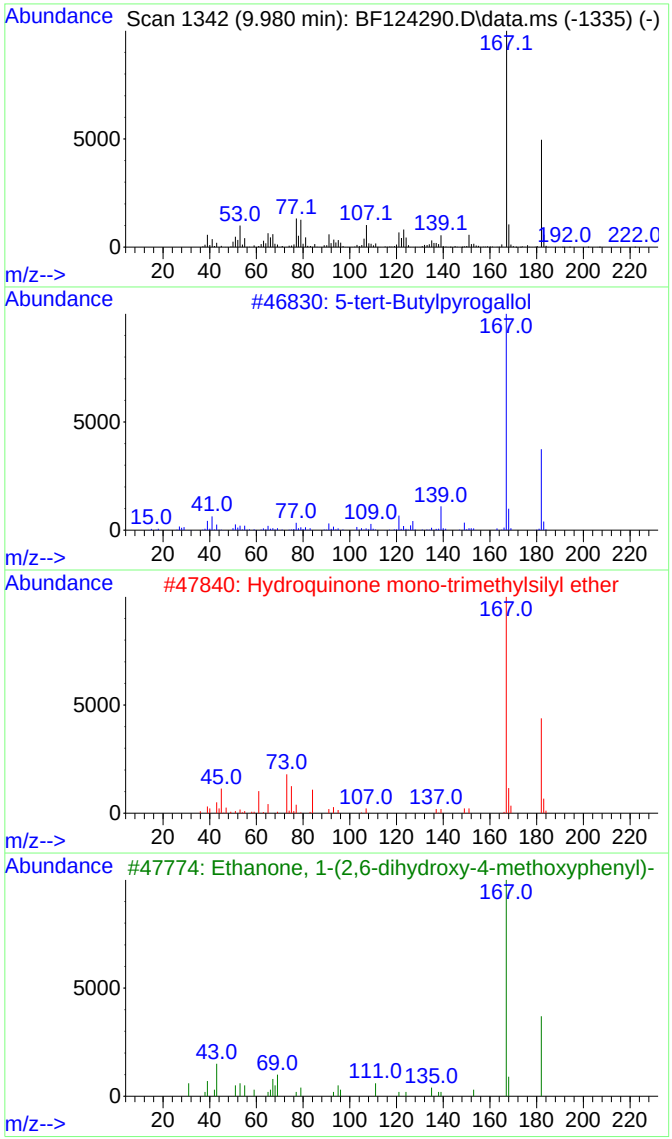
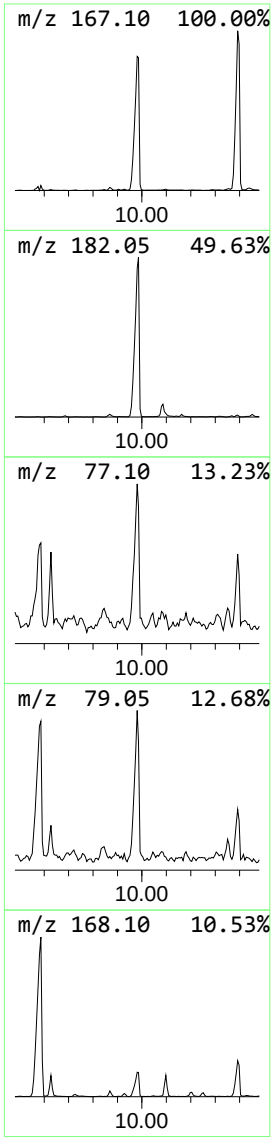
Peak Number 11 5-tert-Butylpyrogallol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.980	303.19 ng	4289240	Acenaphthene-d10	9.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-tert-Butylpyrogallol	182	C10H14O3	020481-17-8	72
2	Hydroquinone mono-trimethylsilyl...	182	C9H14O2Si	017881-87-7	64
3	Ethanone, 1-(2,6-dihydroxy-4-met...	182	C9H10O4	007507-89-3	59
4	Phenol, 3-[(trimethylsilyl)oxy]-	182	C9H14O2Si	017882-01-8	59
5	4,4-Dimethyl-5-methylene-2-allyl...	182	C9H14N2S	037120-29-9	50





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Operator : JU/CG
Sample : M2674-06 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TMR-DS-06-060921

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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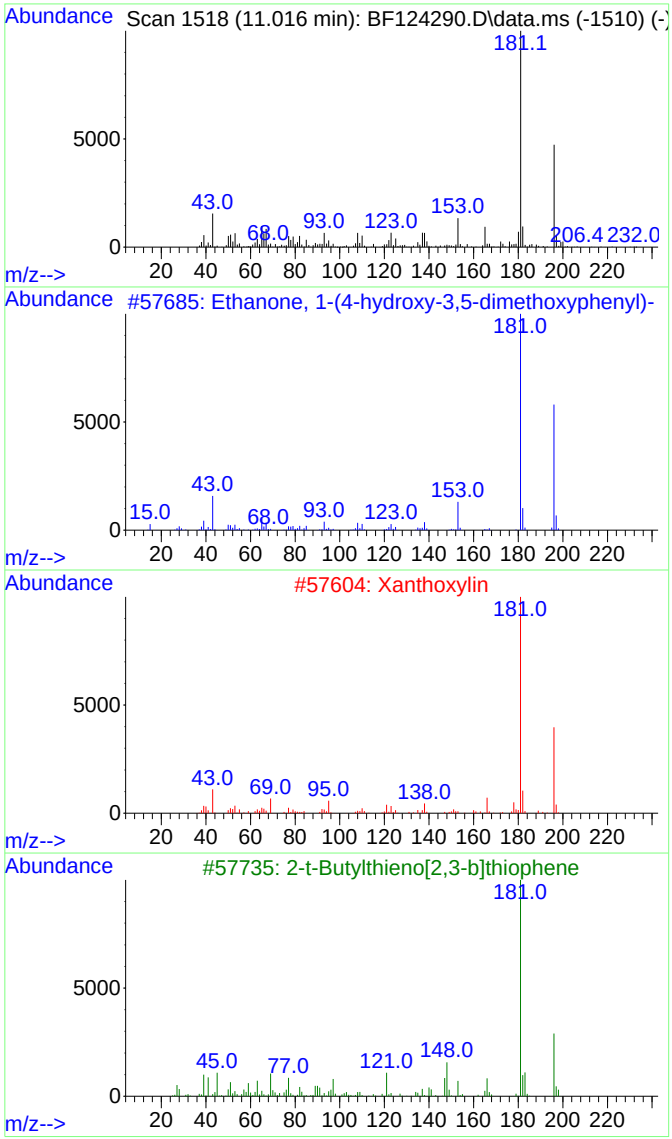
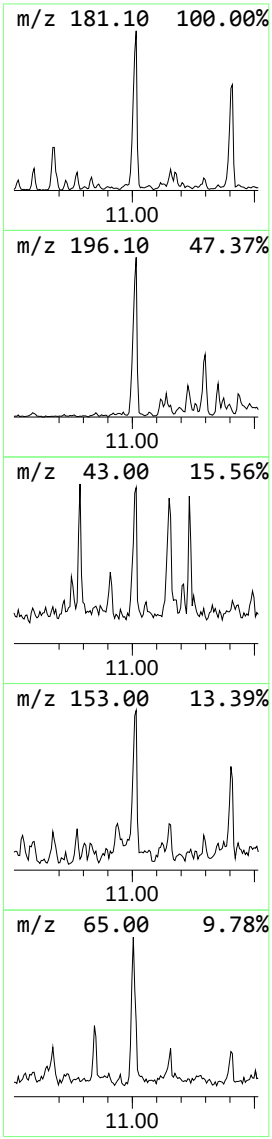
Peak Number 12 Ethanone, 1-(4-hydroxy-3,5-... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.016	58.26 ng	2093940	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanone, 1-(4-hydroxy-3,5-dimet...	196	C10H12O4	002478-38-8	95
2	Xanthoxylin	196	C10H12O4	000090-24-4	72
3	2-t-Butylthieno[2,3-b]thiophene	196	C10H12S2	1000250-49-6	64
4	1-Biphenyl-4-yl-2-(1-phenyl-1H-t...	372	C21H16N4OS	1000300-31-5	47
5	2-Amino-3,5,7,8-tetrahydro-4,6-p...	181	C6H7N5O2	001011-23-0	47





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Sample : M2674-06 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TMR-DS-06-060921

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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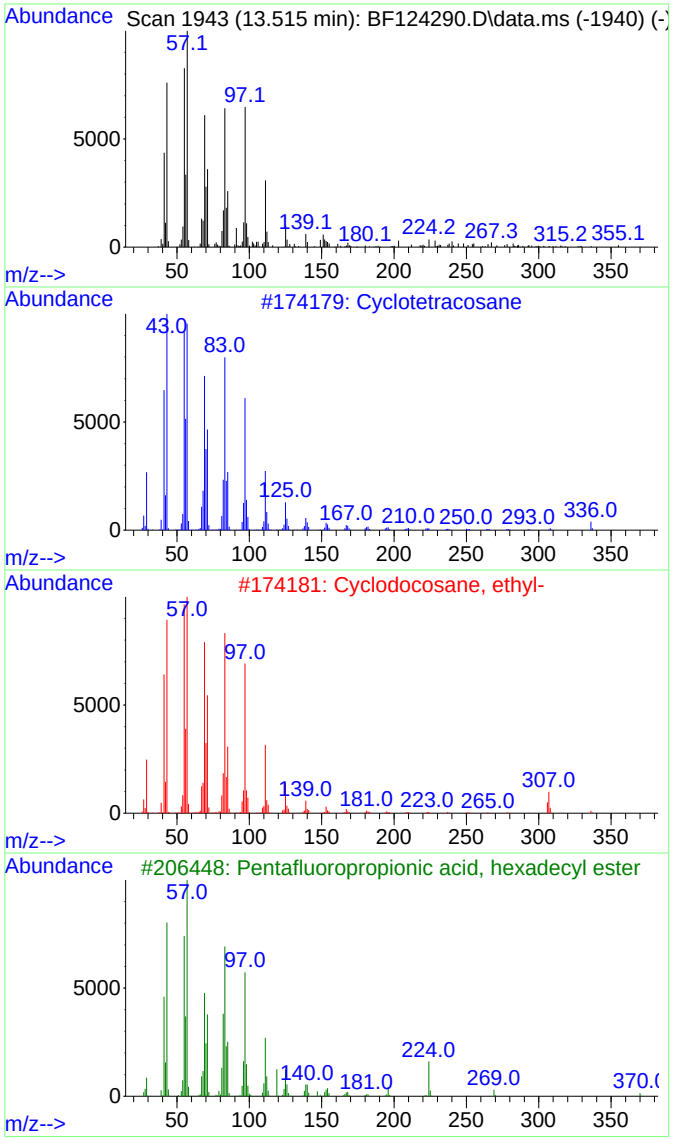
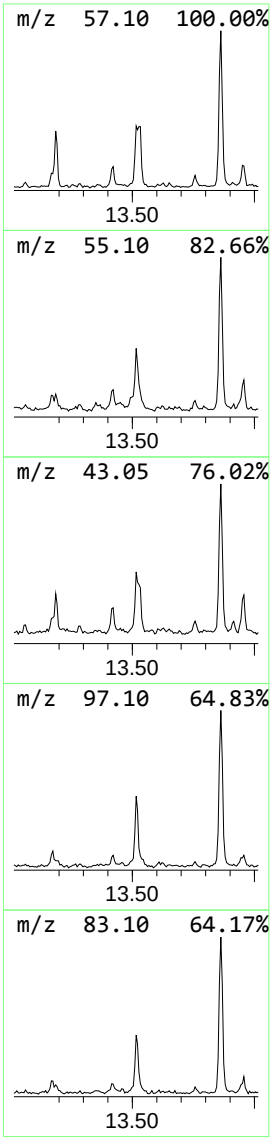
Peak Number 13 Cyclodocosane, ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.515	78.98 ng	1044380	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	95
2	Cyclodocosane, ethyl-	336	C24H48	1000151-22-6	91
3	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
4	1-Tricosene	322	C23H46	018835-32-0	91
5	8-Heptadecene	238	C17H34	002579-04-6	89





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Misc :
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Instrument : BNA_F
ClientSampleId : TMR-DS-06-060921

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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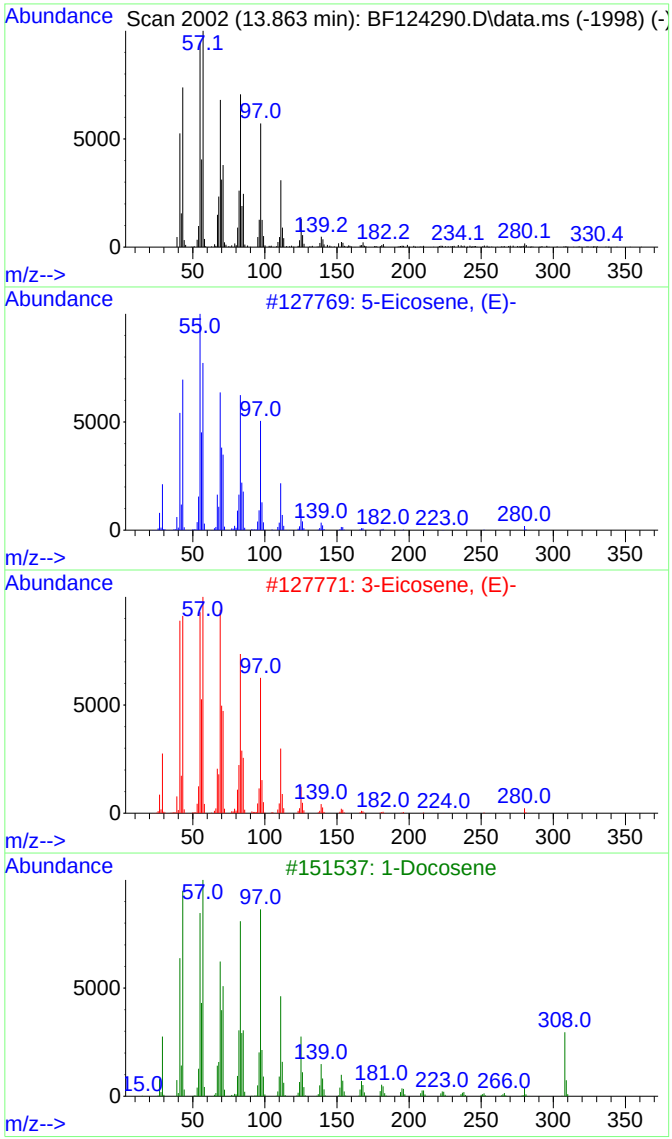
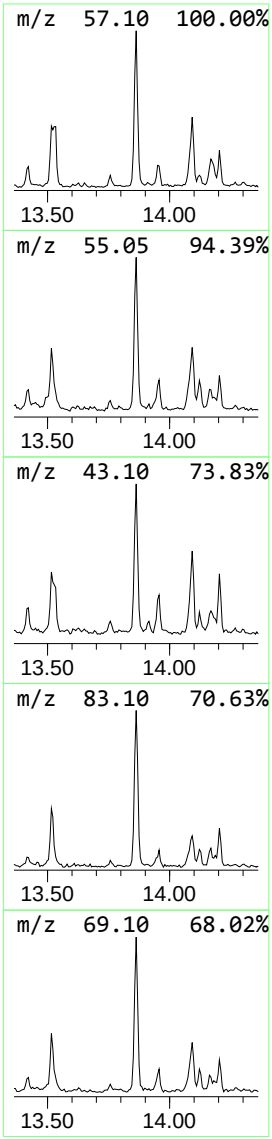
Peak Number 14 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.863	148.24 ng	1960300	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	97
3	1-Docosene	308	C22H44	001599-67-3	95
4	Cycloeicosane	280	C20H40	000296-56-0	94
5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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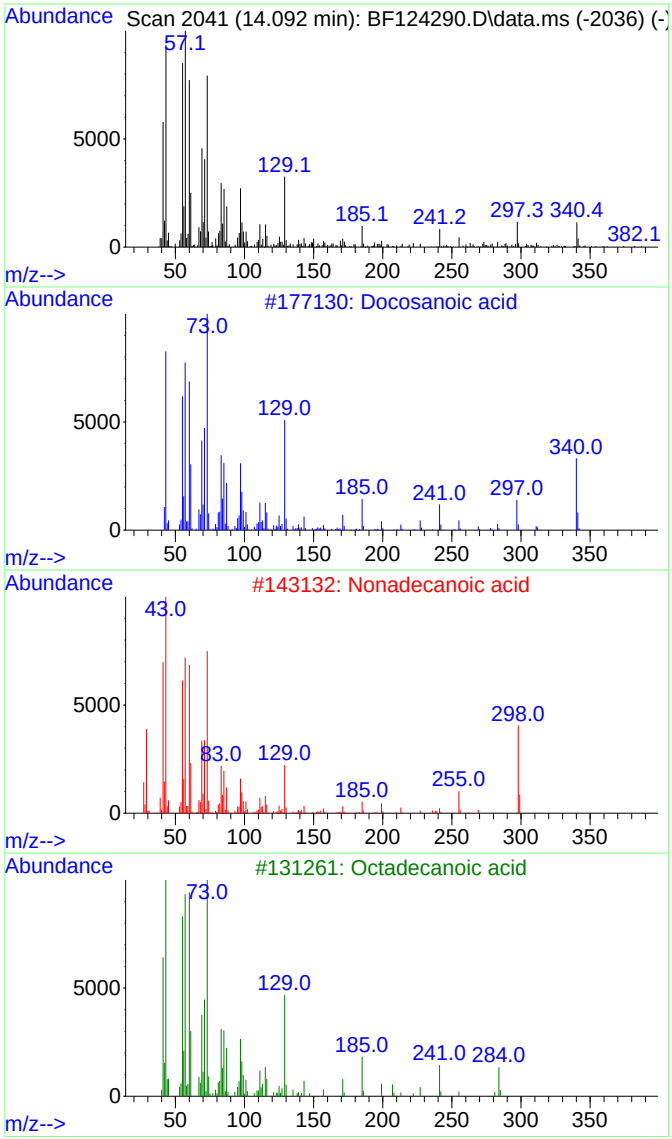
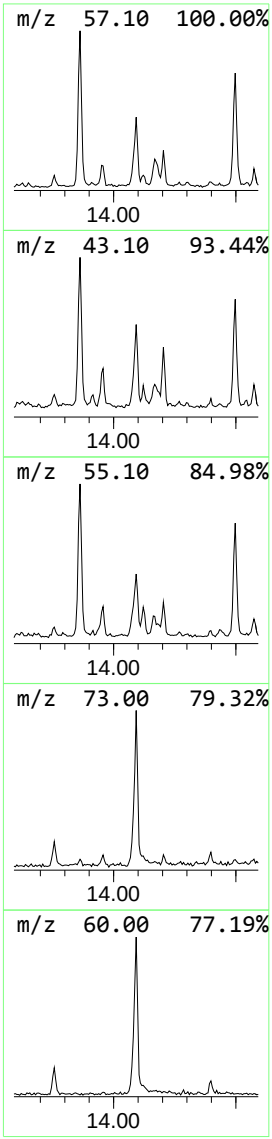
Peak Number 15 Docosanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.092	96.83 ng	1280420	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosanoic acid	340	C22H44O2	000112-85-6	99
2	Nonadecanoic acid	298	C19H38O2	000646-30-0	93
3	Octadecanoic acid	284	C18H36O2	000057-11-4	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	58
5	Undecanoic acid, 10-bromo-	264	C11H21BrO2	018294-93-4	30





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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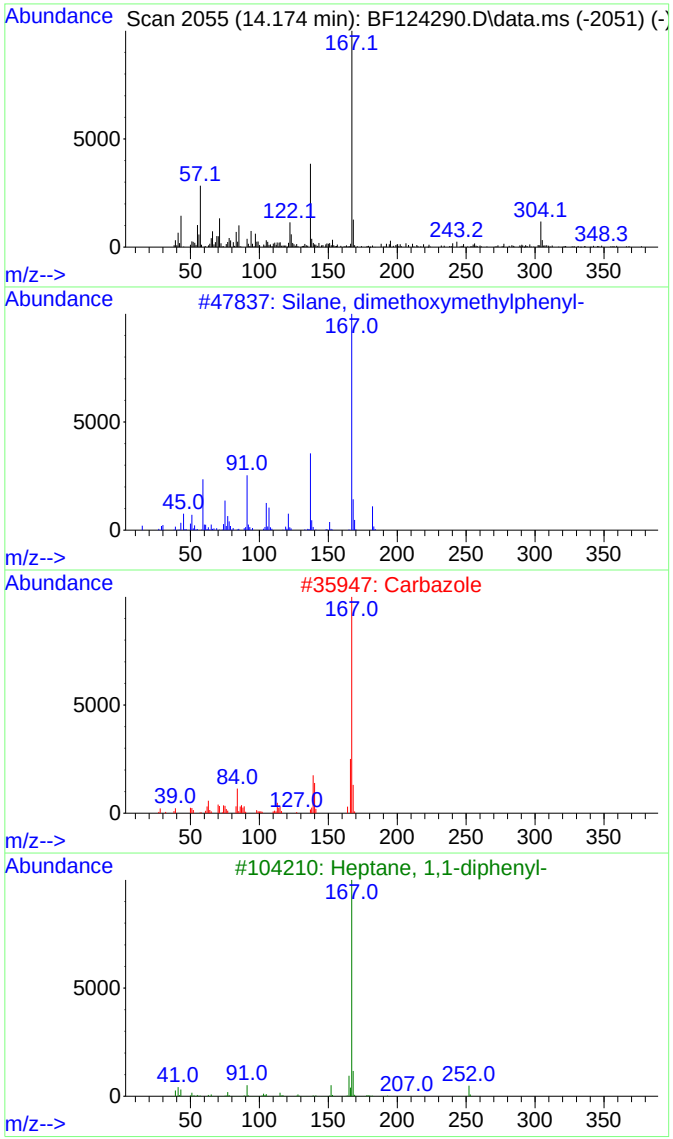
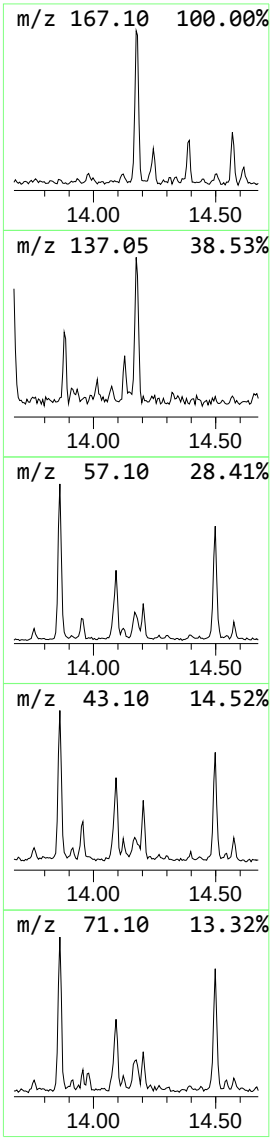
Peak Number 16 unknown14.174 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.174	57.20 ng	756405	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Silane, dimethoxymethylphenyl-	182	C9H14O2Si	003027-21-2	45
2	Carbazole	167	C12H9N	000086-74-8	43
3	Heptane, 1,1-diphenyl-	252	C19H24	001530-05-8	38
4	4H-Pyran-4-one, 2,2'-isopropylid...	320	C17H20O6	033771-01-6	37
5	2,4-Hexadienedioic acid, 3,4-die...	226	C12H18O4	031447-54-8	37





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Data File : BF124290.D
Acq On : 12 Jun 2021 17:14
Operator : JU/CG
Sample : M2674-06 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TMR-DS-06-060921

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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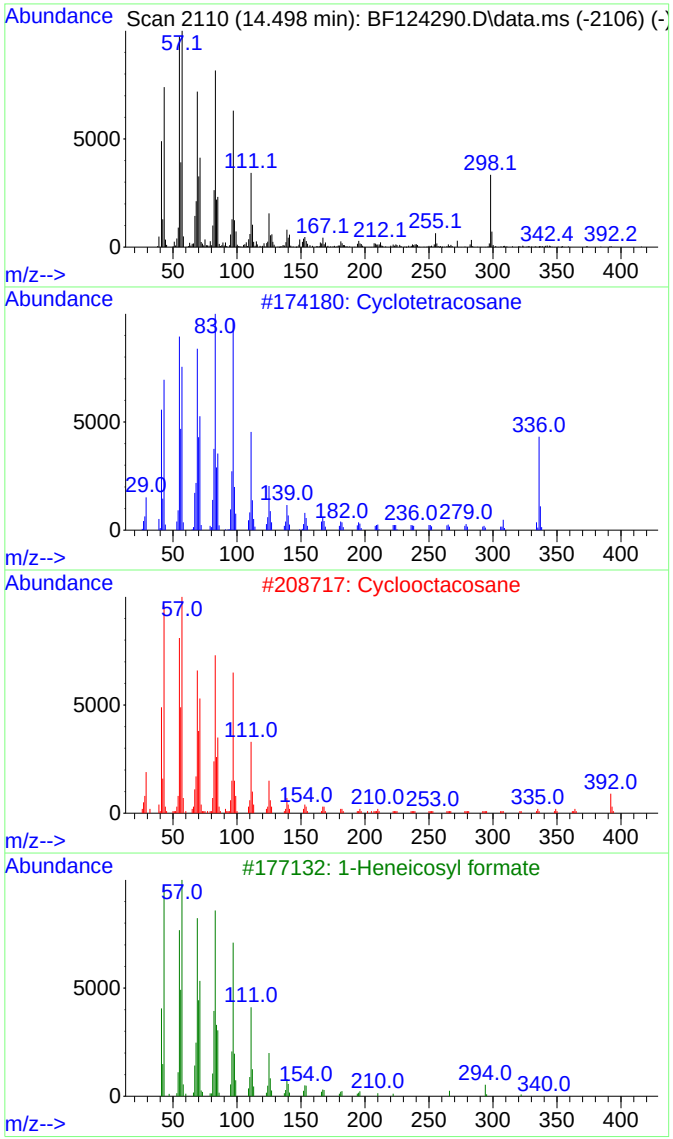
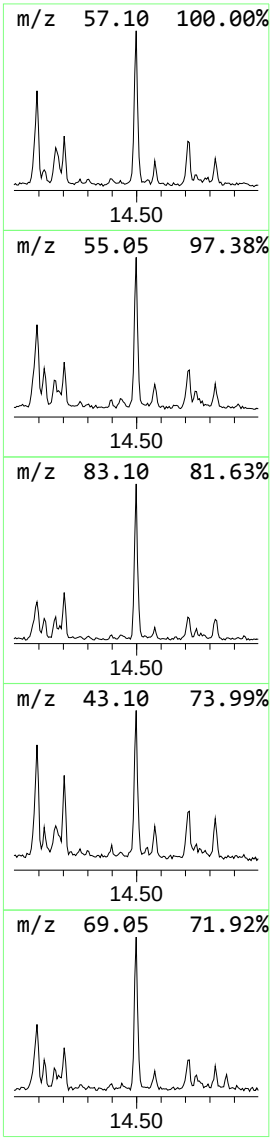
Peak Number 17 Cyclotetracosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.498	126.21 ng	1668910	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	96
2	Cyclooctacosane	392	C28H56	000297-24-5	96
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	95
4	1-Docosene	308	C22H44	001599-67-3	93
5	Behenic alcohol	326	C22H46O	000661-19-8	90





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Data File : BF124290.D
Acq On : 12 Jun 2021 17:14
Operator : JU/CG
Sample : M2674-06 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TMR-DS-06-060921

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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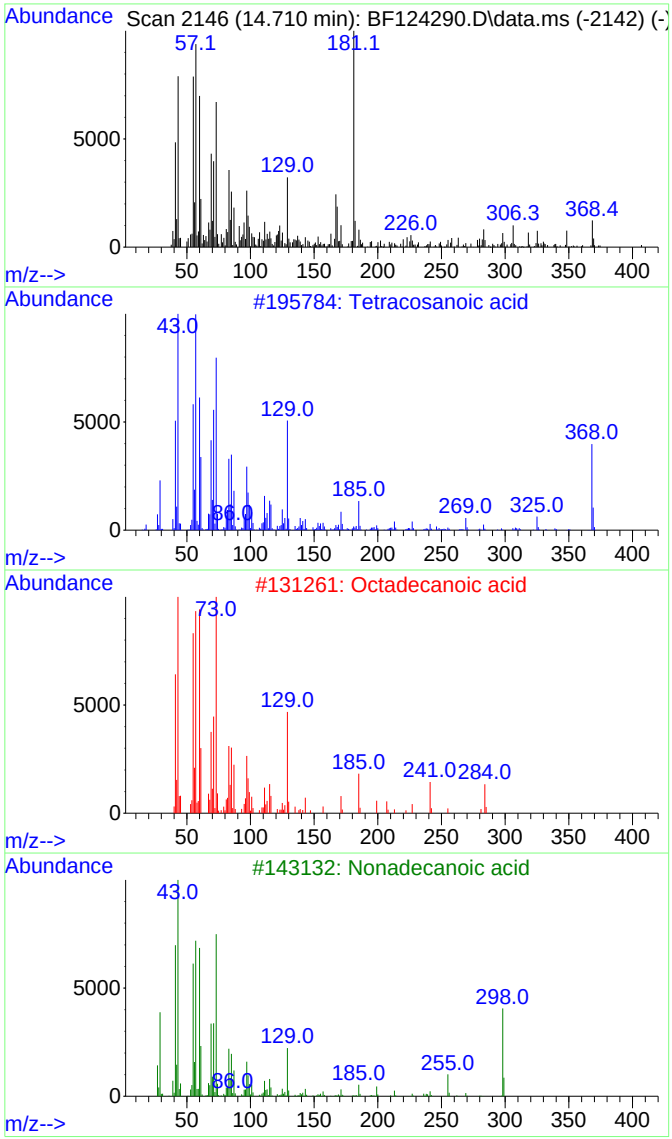
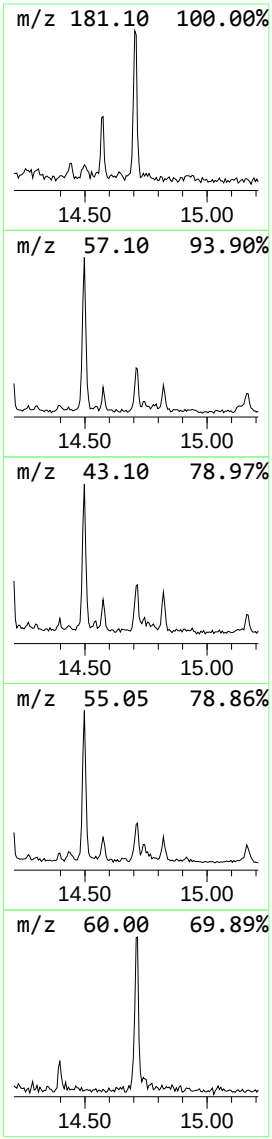
Peak Number 18 Tetracosanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.710	68.86 ng	910633	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosanoic acid	368	C24H48O2	000557-59-5	91
2	Octadecanoic acid	284	C18H36O2	000057-11-4	87
3	Nonadecanoic acid	298	C19H38O2	000646-30-0	64
4	2H-1-Benzopyran-2-one, 4-hydroxy...	298	C17H14O5	004222-00-8	43
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	38





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Data File : BF124290.D
Acq On : 12 Jun 2021 17:14
Operator : JU/CG
Sample : M2674-06 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TMR-DS-06-060921

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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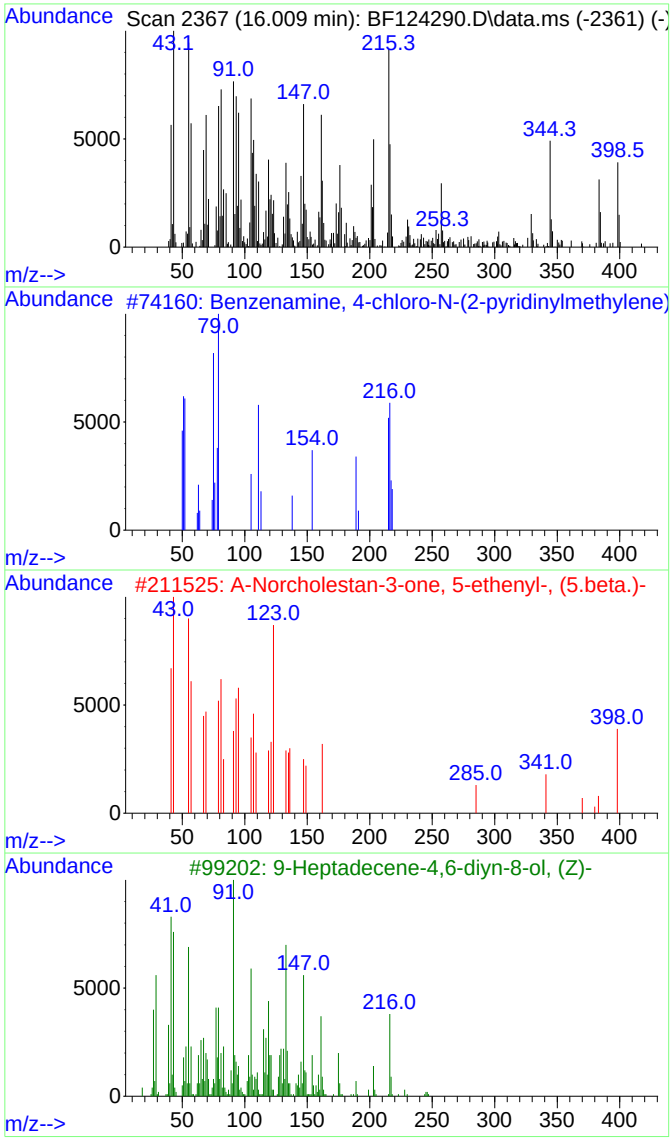
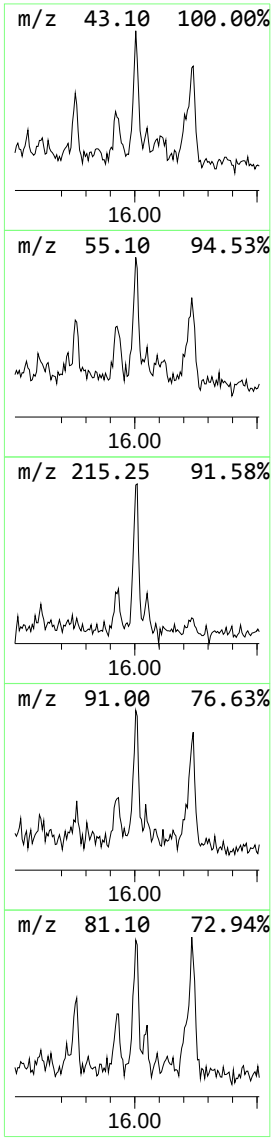
Peak Number 19 Benzenamine, 4-chloro-N-(2-... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.009	44.68 ng	873694	Perylene-d12	15.521

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenamine, 4-chloro-N-(2-pyrid...	216	C12H9ClN2	026825-34-3	56
2	A-Norcholestan-3-one, 5-ethenyl-...	398	C28H46O	019594-90-2	44
3	9-Heptadecene-4,6-diyn-8-ol, (Z)-	246	C17H26O	032768-90-4	18
4	Cyclopent[e]-1,3-oxazine, octahy...	216	C13H16N2O	1000138-92-2	14
5	1-Cycloheptene-3-carboxamide, N-...	215	C14H17NO	1000159-24-4	14





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061221\
Data File : BF124290.D
Acq On : 12 Jun 2021 17:14
Operator : JU/CG
Sample : M2674-06 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TMR-DS-06-060921

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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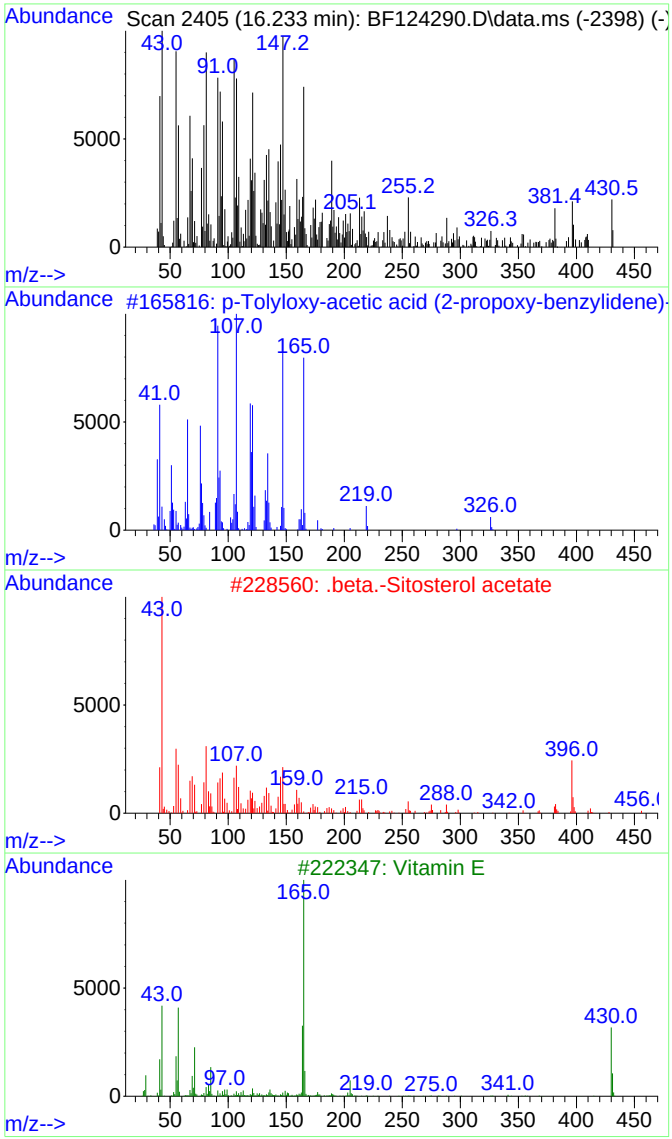
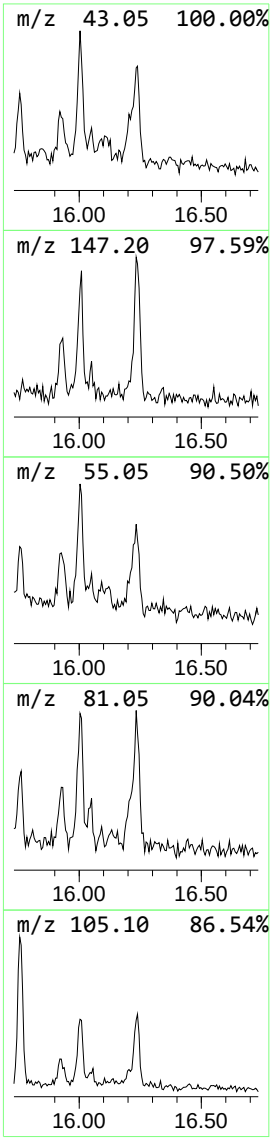
Peak Number 20 unknown16.233 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.233	64.57 ng	1262720	Perylene-d12	15.521

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	p-Tolyloxy-acetic acid (2-propox...	326	C19H22N2O3	1000297-37-9	35
2	.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	27
3	Vitamin E	430	C29H50O2	000059-02-9	25
4	9,19-Cycloergost-24(28)-en-3-ol,...	468	C32H52O2	010376-42-8	20
5	Silane, trimethyl(phenylmethoxy)-	180	C10H16OSi	014642-79-6	15





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061221\
Data File : BF124290.D
Acq On : 12 Jun 2021 17:14
Operator : JU/CG
Sample : M2674-06 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TMR-DS-06-060921

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Benzenemethanol...	7.545	45.0	ng	667700	2	8.128	296847	20.0
Phenol, 2,3-dim...	8.010	55.6	ng	825340	2	8.128	296847	20.0
1H-Benzimidazol...	8.304	78.1	ng	1159640	2	8.128	296847	20.0
Phenol, 2-ethyl...	8.510	71.9	ng	1067040	2	8.128	296847	20.0
Phenol, 4-ethyl...	8.633	122.3	ng	1815850	2	8.128	296847	20.0
Phenol, 2,6-dim...	9.075	323.9	ng	4581700	3	9.892	282940	20.0
Phenol, 2-metho...	9.151	98.1	ng	1387460	3	9.892	282940	20.0
Naphthalene, 2,...	9.480	82.3	ng	1164420	3	9.892	282940	20.0
1,2,3-Trimethox...	9.586	324.4	ng	4589740	3	9.892	282940	20.0
unknown9.627	9.627	50.3	ng	711846	3	9.892	282940	20.0
5-tert-Butylpyr...	9.980	303.2	ng	4289240	3	9.892	282940	20.0
Ethanone, 1-(4-...	11.016	58.3	ng	2093940	4	11.386	718854	20.0
Cyclodocosane, ...	13.515	79.0	ng	1044380	5	14.033	264473	20.0
5-Eicosene, (E)-	13.863	148.2	ng	1960300	5	14.033	264473	20.0
Docosanoic acid	14.092	96.8	ng	1280420	5	14.033	264473	20.0
unknown14.174	14.174	57.2	ng	756405	5	14.033	264473	20.0
Cyclotetracosane	14.498	126.2	ng	1668910	5	14.033	264473	20.0
Tetracosanoic acid	14.710	68.9	ng	910633	5	14.033	264473	20.0
Benzenamine, 4-...	16.009	44.7	ng	873694	6	15.521	391115	20.0
unknown16.233	16.233	64.6	ng	1262720	6	15.521	391115	20.0