LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110321\
Data File : BF126031.D
Acq On : 3 Nov 2021 21:27
Operator : JU/CG
Sample : M4427-08 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FDR-BH-2-20211029-6.5-7

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-BF110321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126031.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.451	568	572	576	rBV	888031	795784	9.11%	0.547%
2	6.469	741	745	752	rBV	907249	839675	9.61%	0.577%
3	6.851	806	810	813	rBV	1133859	881125	10.08%	0.605%
4	7.380	897	900	902	rBV	149800	162422	1.86%	0.112%
5	7.404	902	904	906	rVV	601248	535569	6.13%	0.368%
6	7.457	910	913	916	rVB3	136784	152318	1.74%	0.105%
7	7.798	967	971	974	rBV4	143993	196713	2.25%	0.135%
8	7.945	990	996	1000	rBV	182671	289404	3.31%	0.199%
9	8.133	1024	1028	1034	rBV	1379699	1198574	13.72%	0.823%
10	8.186	1034	1037	1040	rVB3	99380	131596	1.51%	0.090%
11	8.269	1048	1051	1053	rBV2	139623	168208	1.93%	0.116%
12	8.292	1053	1055	1059	rVV2	248868	339245	3.88%	0.233%
13	8.339	1060	1063	1065	rVV	280958	273118	3.13%	0.188%
14	8.375	1066	1069	1072	rVB2	231423	254980	2.92%	0.175%
15	8.469	1082	1085	1087	rBV2	165644	196068	2.24%	0.135%
16	8.522	1090	1094	1096	rBV2	493114	566488	6.48%	0.389%
17	8.551	1096	1099	1102	rBV	284480	297850	3.41%	0.205%
18	8.622	1108	1111	1114	rBV3	274403	280006	3.20%	0.192%
19	8.657	1114	1117	1119	rBV	2002105	1544016	17.67%	1.061%
20	8.680	1119	1121	1122	rVB	247466	173480	1.99%	0.119%
21	8.716	1125	1127	1129	rBV3	577524	655871	7.51%	0.450%
22	8.780	1136	1138	1141	rVB2	542253	503999	5.77%	0.346%
23	8.822	1141	1145	1148	rBV4	696755	949974	10.87%	0.652%
24	8.898	1148	1158	1162	rBV3	1167565	2690752	30.79%	1.848%
25	8.939	1162	1165	1166	rBV2	386580	418629	4.79%	0.288%
26	9.063	1182	1186	1189	rBV3	922071	1150037	13.16%	0.790%
27	9.092	1189	1191	1193	rBV3	356082	434366	4.97%	0.298%
28	9.122	1193	1196	1199	rVV	1944750	2367588	27.10%	1.626%
29	9.163	1201	1203	1206	rVV	944178	906800	10.38%	0.623%
30	9.192	1206	1208	1209	rVV	518189	415147	4.75%	0.285%
31	9.210	1209	1211	1214	rVB	891194	617122	7.06%	0.424%
32	9.245	1215	1217	1219	rBV3	476437	417080	4.77%	0.286%
33	9.327	1229	1231	1232	rBV	575344	369678	4.23%	0.254%
34	9.369	1236	1238	1240	rVV2	645066	541269	6.19%	0.372%
35	9.410	1242	1245	1249	rVB2	2838431	3231387	36.98%	2.220%
36	9.463	1252	1254	1256	rBV2	981748	872090	9.98%	0.599%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110321\
Data File : BF126031.D
Acq On : 3 Nov 2021 21:27
Operator : JU/CG
Sample : M4427-08 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FDR-BH-2-20211029-6.5-7

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-BF110321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	9.569	1270	1272	1274	rVB2	654151	478975	5.48%	0.329%
38	9.616	1277	1280	1283	rBV2	1452162	1637030	18.73%	1.124%
39	9.645	1283	1285	1287	rVV2	507192	505597	5.79%	0.347%
40	9.698	1291	1294	1297	rVB	593986	576789	6.60%	0.396%
41	9.727	1297	1299	1301	rBV2	387740	432523	4.95%	0.297%
42	9.769	1304	1306	1307	rBV	1114868	837003	9.58%	0.575%
43	9.857	1319	1321	1323	rBV2	621007	578252	6.62%	0.397%
44	9.886	1324	1326	1333	rVB3	1212058	1722457	19.71%	1.183%
45	9.939	1333	1335	1337	rBV2	373362	448842	5.14%	0.308%
46	9.969	1338	1340	1343	rVB	844424	772949	8.85%	0.531%
47	10.098	1360	1362	1365	rBV3	786385	812580	9.30%	0.558%
48	10.127	1365	1367	1371	rVB	1076469	1343329	15.37%	0.923%
49	10.304	1393	1397	1401	rBV3	1116731	1718976	19.67%	1.181%
50	10.386	1408	1411	1414	rVB2	2593519	2520872	28.85%	1.731%
51	10.433	1416	1419	1426	rVB3	3429874	4372093	50.04%	3.003%
52	10.557	1437	1440	1441	rBV	2676186	2495419	28.56%	1.714%
53	10.574	1441	1443	1445	rVB	2539973	1856206	21.24%	1.275%
54	10.598	1445	1447	1452	rBV2	2816817	2406846	27.54%	1.653%
55	10.639	1452	1454	1457	rBV2	1993068	2368205	27.10%	1.627%
56	10.704	1463	1465	1467	rVB	2302305	1706758	19.53%	1.172%
57	10.763	1471	1475	1479	rBV	8001727	8737995	100.00%	6.002%
58	10.798	1479	1481	1484	rVB2	2404988	1993098	22.81%	1.369%
59	10.851	1487	1490	1492	rBV	6189578	5533108	63.32%	3.800%
60	10.916	1497	1501	1505	rBV	7489950	7955010	91.04%	5.464%
61	10.957	1505	1508	1510	rBV	2556965	2595812	29.71%	1.783%
62	11.045	1520	1523	1525	rBV	2024105	2240829	25.64%	1.539%
63	11.133	1536	1538	1540	rVB	1137660	877864	10.05%	0.603%
64	11.157	1540	1542	1545	rBV	1332040	1316971	15.07%	0.905%
65	11.192	1545	1548	1551	rBV	2320735	2286932	26.17%	1.571%
66	11.251	1554	1558	1561	rVV2	2961714	4148144	47.47%	2.849%
67	11.280	1561	1563	1568	rVB	1969124	1715928	19.64%	1.179%
68	11.339	1569	1573	1577	rBV2	4694640	7699841	88.12%	5.289%
69	11.380	1577	1580	1581	rBV3	1087000	1073988	12.29%	0.738%
70	11.404	1581	1584	1586	rVB	2942107	2244931	25.69%	1.542%
71	11.439	1586	1590	1593	rBV	3027491	3408900	39.01%	2.341%
72	11.474	1593	1596	1600	rBV2	2097483	2657148	30.41%	1.825%
73	11.545	1606	1608	1610	rBV	1407085	1127999	12.91%	0.775%
74	11.568	1610	1612	1616	rVB2	2567554	3190372	36.51%	2.191%
75	11.615	1617	1620	1623	rBV	3939630	4290252	49.10%	2.947%
76	11.698	1630	1634	1639	rBV2	4189637	8691166	99.46%	5.970%

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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
FDR-BH-2-20211029-6.5-7

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
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Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	11.745	1640	1642	1645	rVB	3248075	3244287	37.13%	2.228%
78	11.792	1645	1650	1652	rBV	4056641	6236321	71.37%	4.283%
79	11.839	1656	1658	1660	rBV	3558105	3370947	38.58%	2.315%
80	12.086	1698	1700	1703	rBV2	1784690	1400454	16.03%	0.962%
81	12.392	1750	1752	1754	rBV2	1189531	1281611	14.67%	0.880%
82	15.480	2275	2277	2281	rVB	807821	860475	9.85%	0.591%

Sum of corrected areas: 145590512

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110321\
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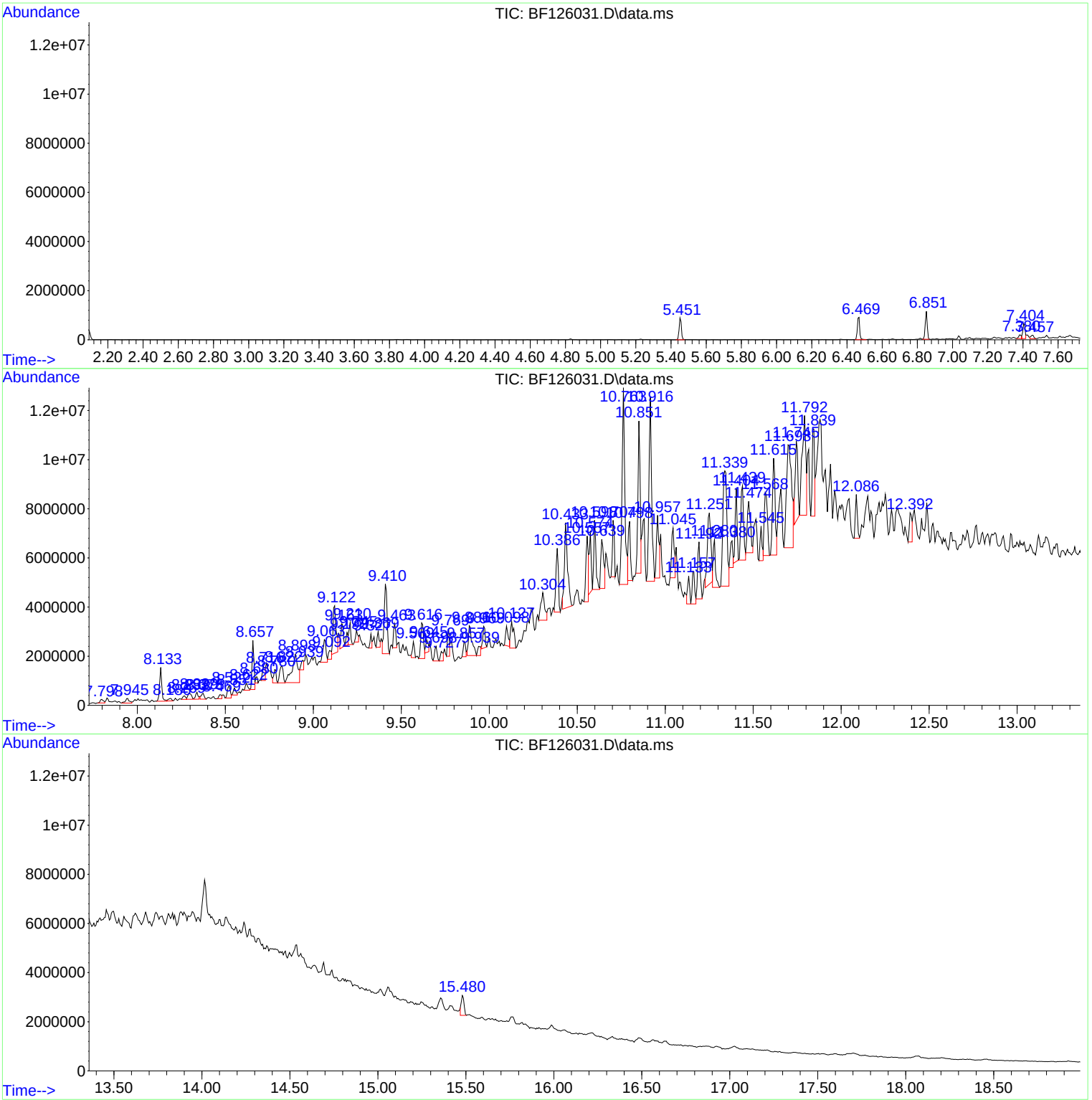
Instrument :
BNA_F
ClientSampleId :
FDR-BH-2-20211029-6.5-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.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\BF110321\
Data File : BF126031.D
Acq On : 3 Nov 2021 21:27
Operator : JU/CG
Sample : M4427-08 5X
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ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
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FDR-BH-2-20211029-6.5-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

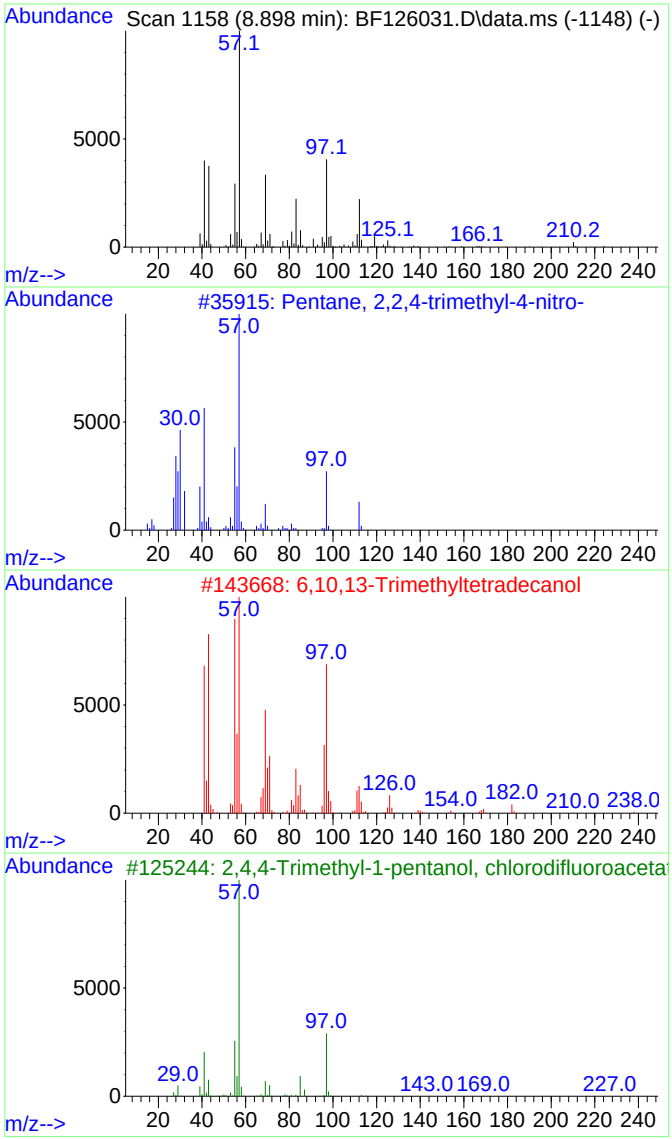
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

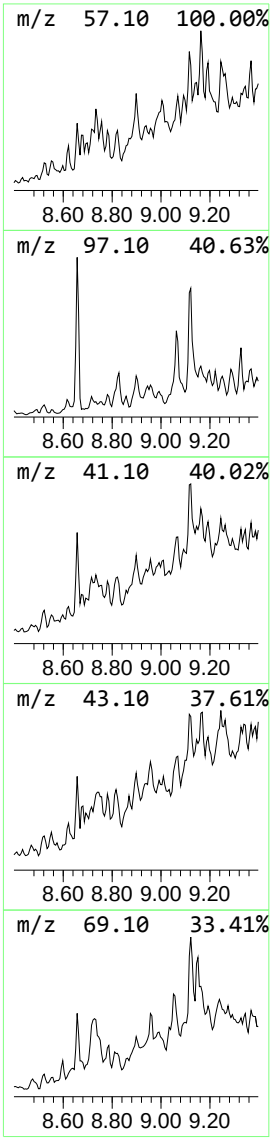
****

Peak Number 1 Pentane, 2,2,4-trimethyl-4-... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.898	44.90 ng	2690750	Naphthalene-d8	8.133

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,2,4-trimethyl-4-nitro-	159	C8H17NO2	005342-78-9	53
2	6,10,13-Trimethyltetradecanol	256	C17H36O	1000131-71-0	40
3	2,4,4-Trimethyl-1-pentanol, chlo...	242	C10H17ClF2O2	1000447-27-2	38
4	1-Pentene, 2,4,4-trimethyl-	112	C8H16	000107-39-1	35
5	1-Pentene, 4,4-dimethyl-	98	C7H14	000762-62-9	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110321\
Data File : BF126031.D
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Sample : M4427-08 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FDR-BH-2-20211029-6.5-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

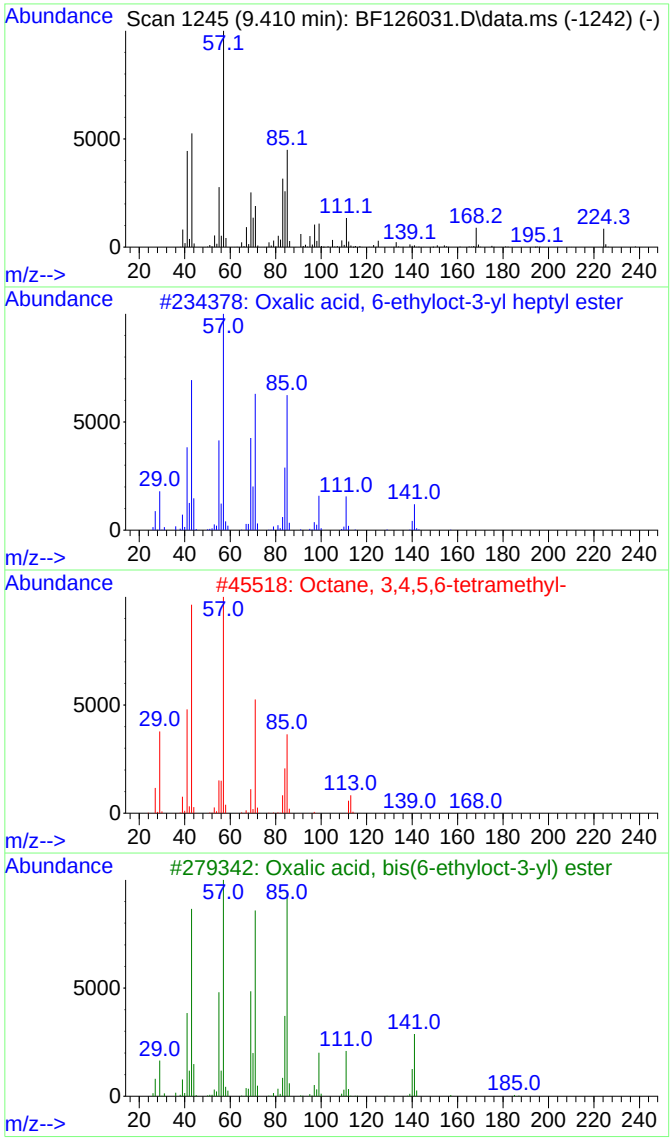
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

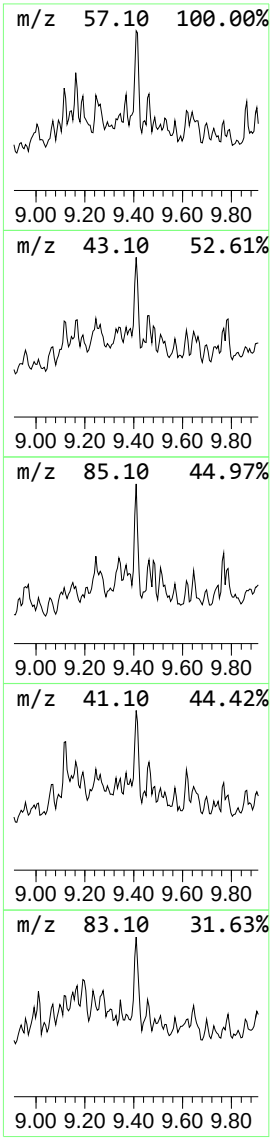
****

Peak Number 2 unknown9.410 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.410	37.52 ng	3231390	Acenaphthene-d10	9.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, 6-ethyloct-3-yl hep...	328	C19H36O4	1000309-34-5	45
2	Octane, 3,4,5,6-tetramethyl-	170	C12H26	062185-21-1	43
3	Oxalic acid, bis(6-ethyloct-3-yl...	370	C22H42O4	1000309-34-6	38
4	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	38
5	Sulfurous acid, hexyl heptyl ester	264	C13H28O3S	1000309-12-9	38





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

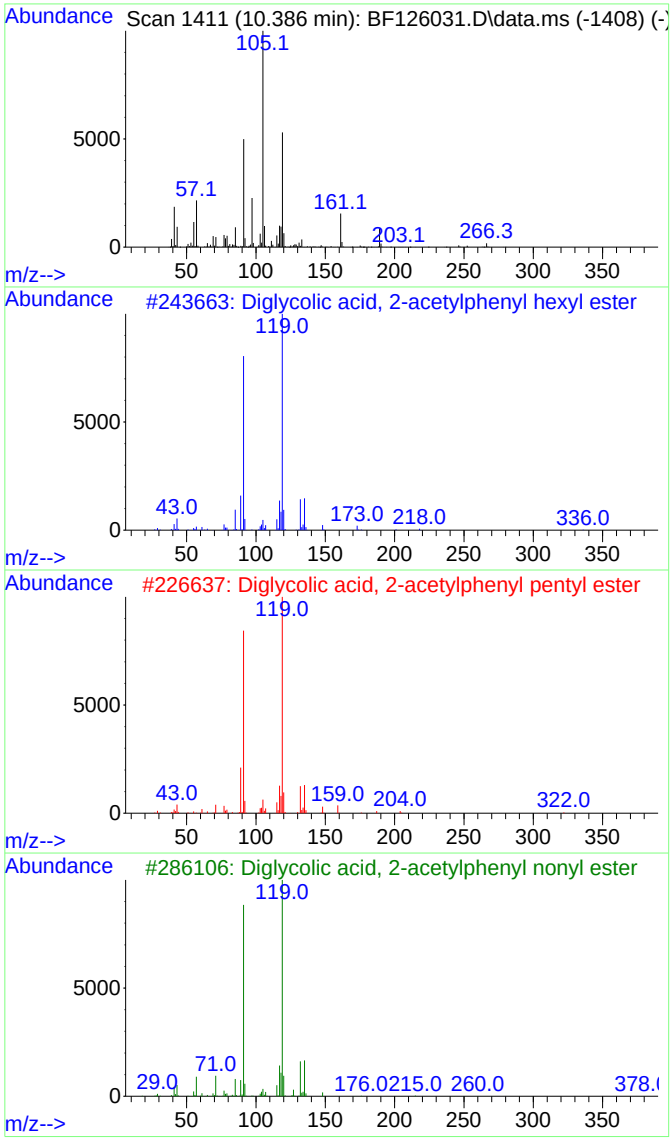
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

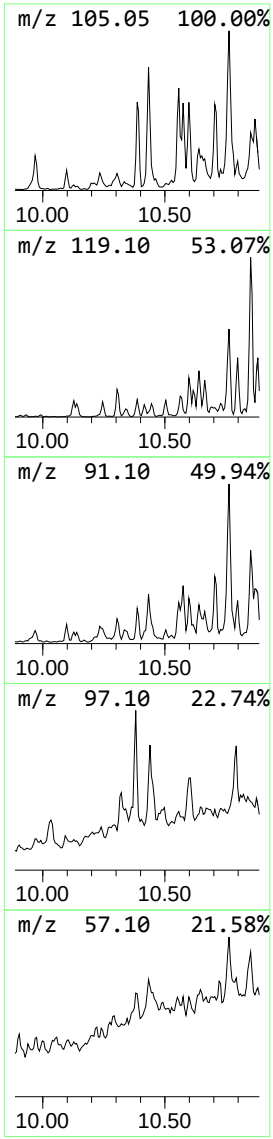
****

Peak Number 3 unknown10.386 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.386	29.27 ng	2520870	Acenaphthene-d10	9.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diglycolic acid, 2-acetylphenyl ...	336	C18H24O6	1000382-72-2	38
2	Diglycolic acid, 2-acetylphenyl ...	322	C17H22O6	1000382-72-0	35
3	Diglycolic acid, 2-acetylphenyl ...	378	C21H30O6	1000382-72-5	32
4	Benzene, (1,1,2-trimethylpropyl)-	162	C12H18	026356-11-6	30
5	N-(2-Phenylethenyl)acetamide	161	C10H11NO	1000305-37-3	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110321\
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Instrument :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

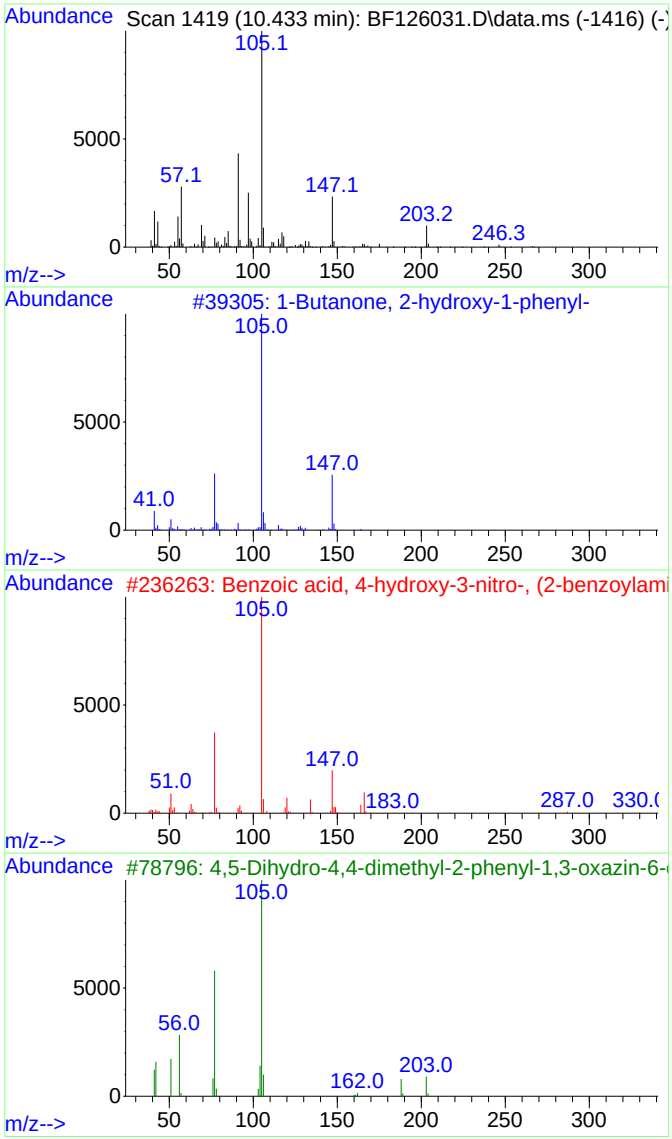
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

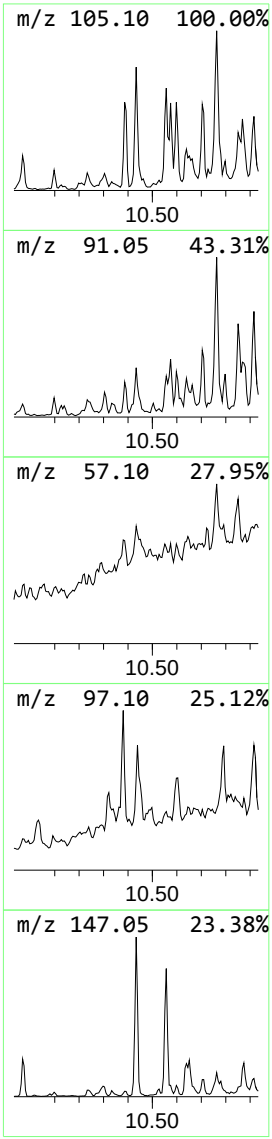
****

Peak Number 4 unknown10.433 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.433	50.77 ng	4372090	Acenaphthene-d10	9.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanone, 2-hydroxy-1-phenyl-	164	C10H12O2	016183-46-3	32
2	Benzoic acid, 4-hydroxy-3-nitro-...	330	C16H14N2O6	346661-98-1	17
3	4,5-Dihydro-4,4-dimethyl-2-pheny...	203	C12H13NO2	029637-55-6	16
4	Benzoic acid, 3,4-dichlorophenyl...	266	C13H8Cl2O2	1000357-80-2	14
5	Hydratropic acid, undec-2-en-1-y...	302	C20H30O2	1000406-96-0	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110321\
Data File : BF126031.D
Acq On : 3 Nov 2021 21:27
Operator : JU/CG
Sample : M4427-08 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FDR-BH-2-20211029-6.5-7

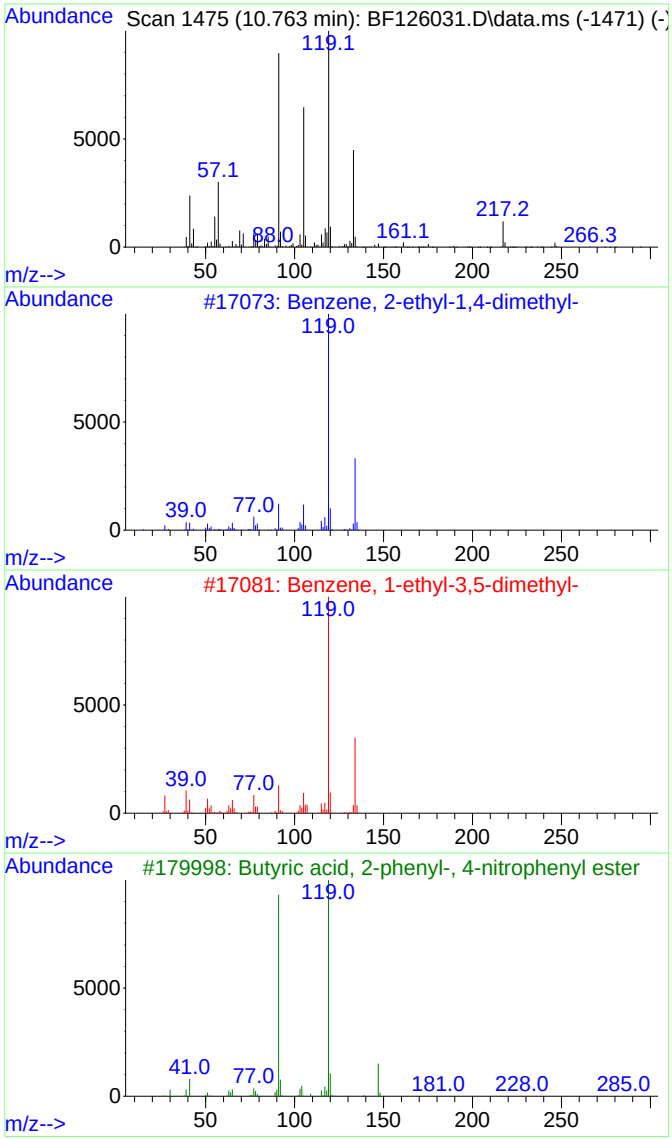
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

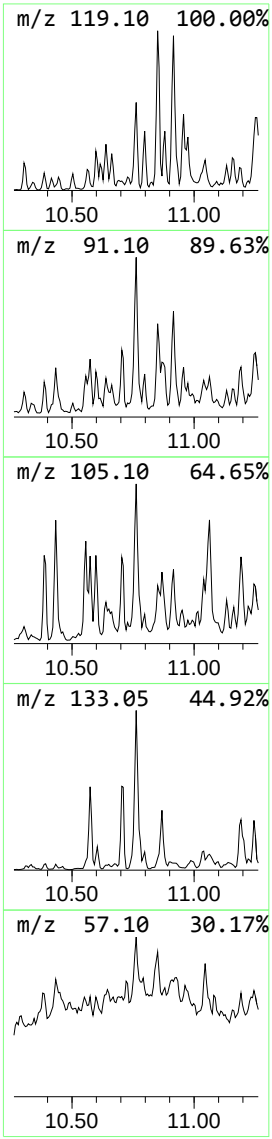
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.763	162.72 ng	8738000	Phenanthrene-d10	11.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	53
2	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	50
3	Butyric acid, 2-phenyl-, 4-nitro...	285	C16H15NO4	1000406-87-5	50
4	Diglycolic acid, 2-acetylphenyl ...	280	C14H16O6	1000382-71-6	50
5	Benzene, (1,1-dimethyldecyl)-	246	C18H30	027854-40-6	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110321\
Data File : BF126031.D
Acq On : 3 Nov 2021 21:27
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Sample : M4427-08 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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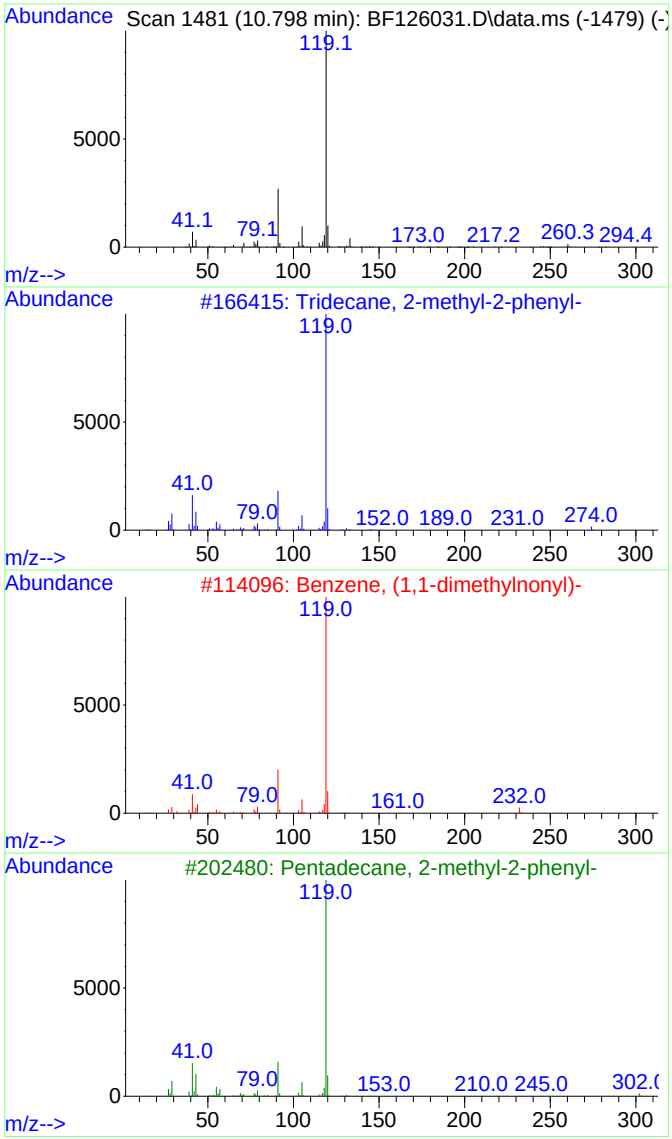
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

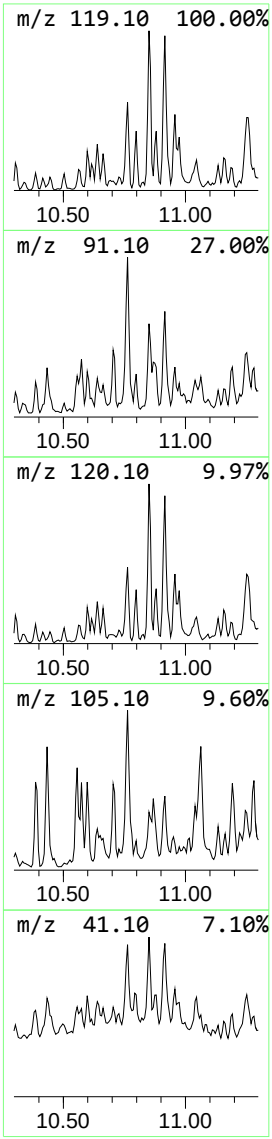
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, (1,1-dimethylnonyl)- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.798	37.12 ng	1993100	Phenanthrene-d10	11.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 2-methyl-2-phenyl-	274	C20H34	027854-41-7	78
2	Benzene, (1,1-dimethylnonyl)-	232	C17H28	055191-25-8	78
3	Pentadecane, 2-methyl-2-phenyl-	302	C22H38	029138-94-1	78
4	Benzene, (1,1,4,6,6-pentamethylh...	246	C18H30	055134-07-1	78
5	Cumene hydroperoxide, TMS deriva...	224	C12H20O2Si	018057-16-4	78





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Sample : M4427-08 5X
Misc :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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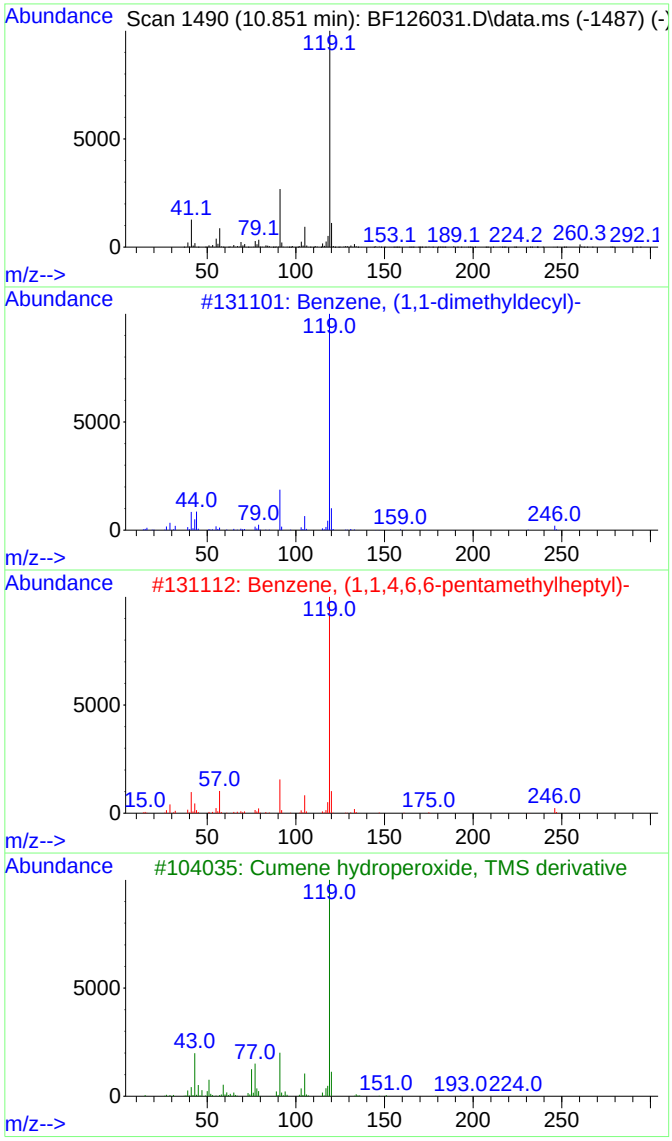
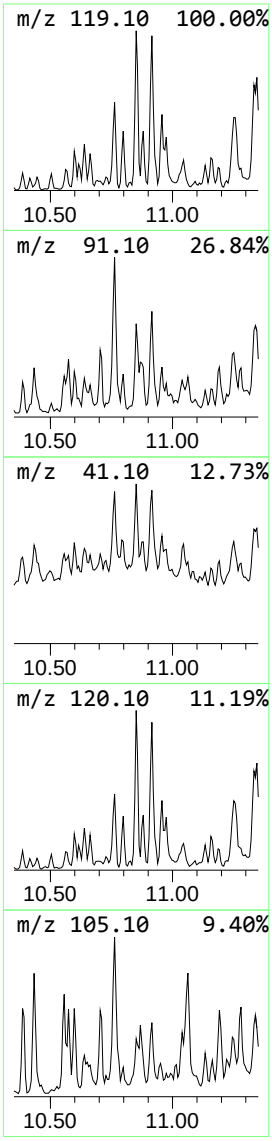
Peak Number 7 Benzene, (1,1,4,6,6-pentame... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.851	103.04 ng	5533110	Phenanthrene-d10	11.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1,1-dimethyldecyl)-	246	C18H30	027854-40-6	78
2	Benzene, (1,1,4,6,6-pentamethylh...	246	C18H30	055134-07-1	78
3	Cumene hydroperoxide, TMS deriva...	224	C12H20O2Si	018057-16-4	78
4	Benzene, (1,1-dimethylnonyl)-	232	C17H28	055191-25-8	78
5	Phenyl iso-butyl methylcarbinyl ...	220	C14H20O2	1000285-48-0	78





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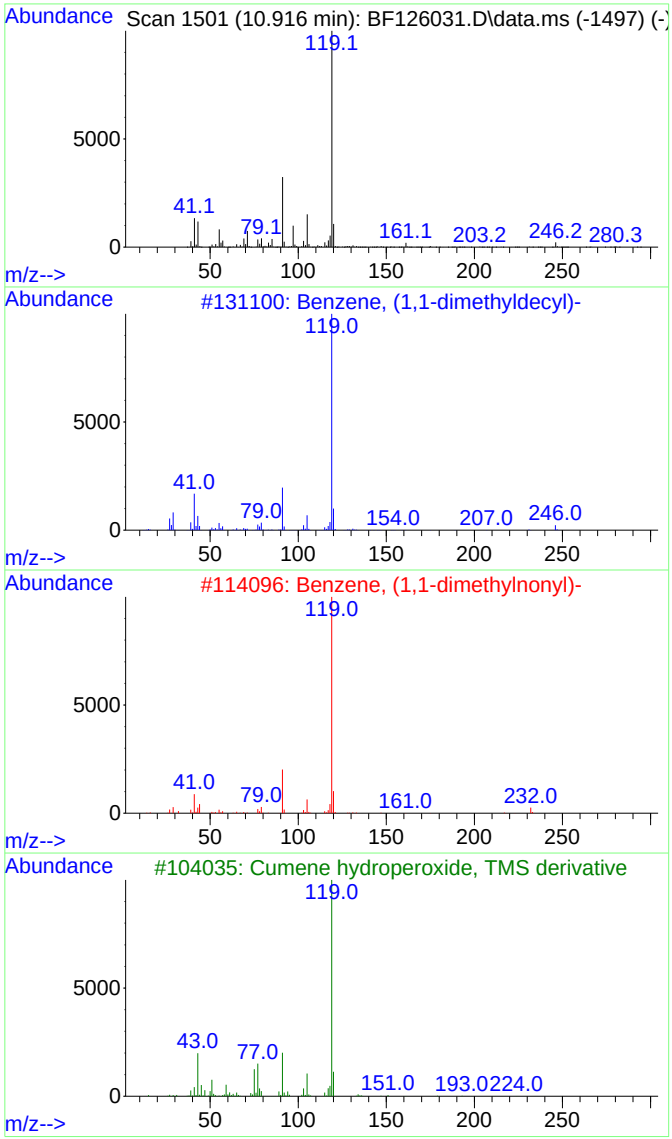
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

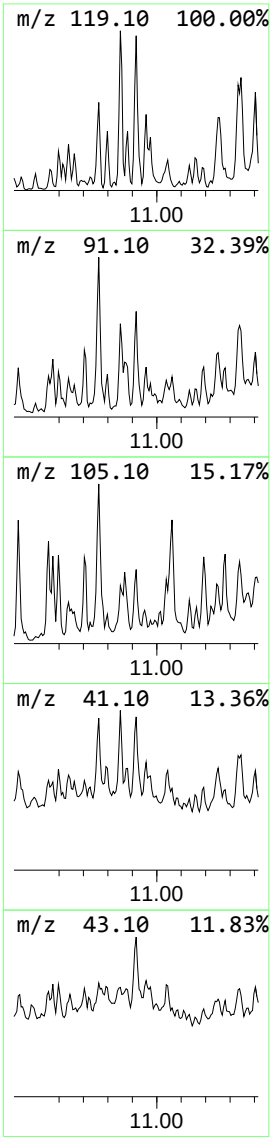
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Cumene hydroperoxide, TMS d... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.916	148.14 ng	7955010	Phenanthrene-d10	11.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1,1-dimethyldecyl)-	246	C18H30	027854-40-6	81
2	Benzene, (1,1-dimethylnonyl)-	232	C17H28	055191-25-8	64
3	Cumene hydroperoxide, TMS deriva...	224	C12H20O2Si	018057-16-4	64
4	Benzene, 1-(1,5-dimethylhexyl)-4...	204	C15H24	001461-02-5	64
5	2-Hexanone, 5-methyl-5-phenyl-	190	C13H18O	014128-61-1	59





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

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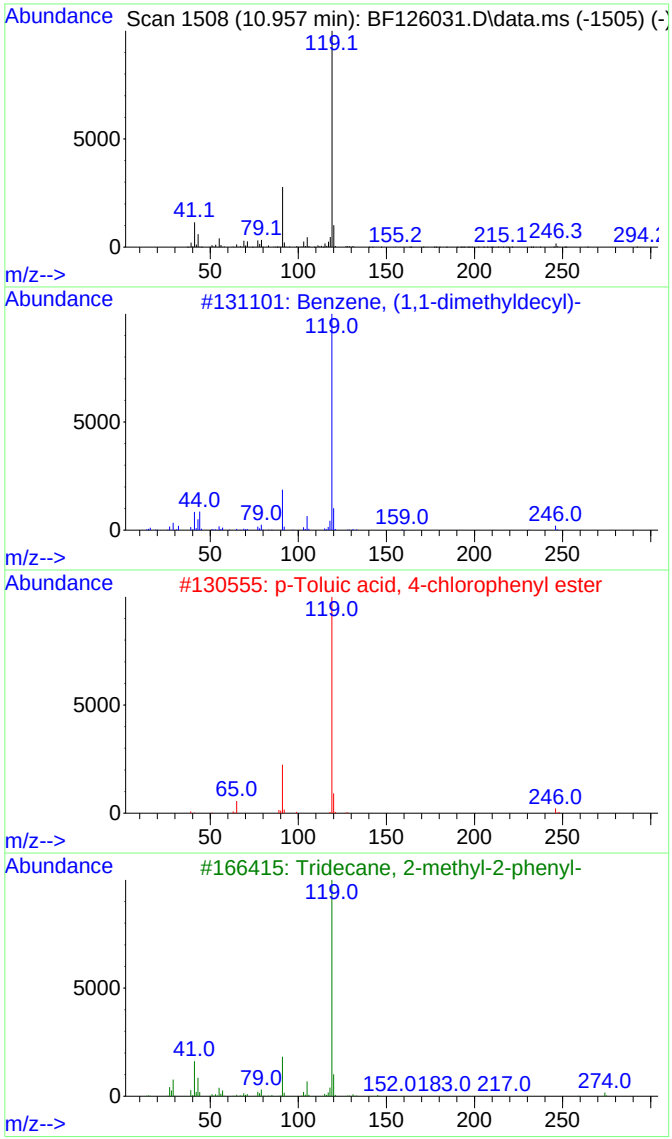
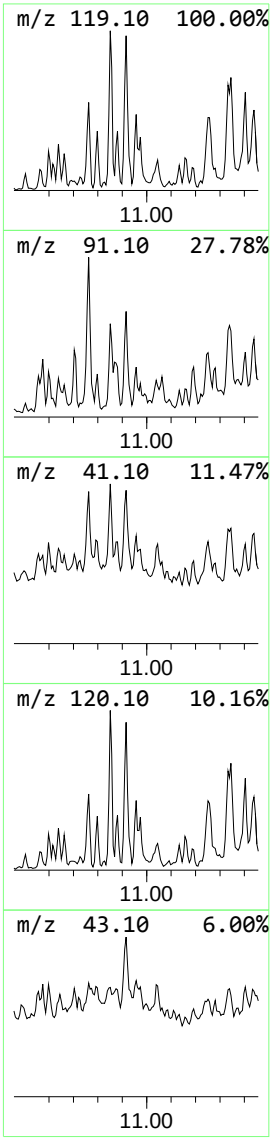
Peak Number 9 Benzene, (1,1-dimethyldecyl)- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.957	48.34 ng	2595810	Phenanthrene-d10	11.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1,1-dimethyldecyl)-	246	C18H30	027854-40-6	90
2	p-Toluic acid, 4-chlorophenyl ester	246	C14H11ClO2	1010307-76-5	86
3	Tridecane, 2-methyl-2-phenyl-	274	C20H34	027854-41-7	83
4	p-Menthane, 2,3-dibromo-8-phenyl-	372	C16H22Br2	1000152-61-6	83
5	Pentadecane, 2-methyl-2-phenyl-	302	C22H38	029138-94-1	83





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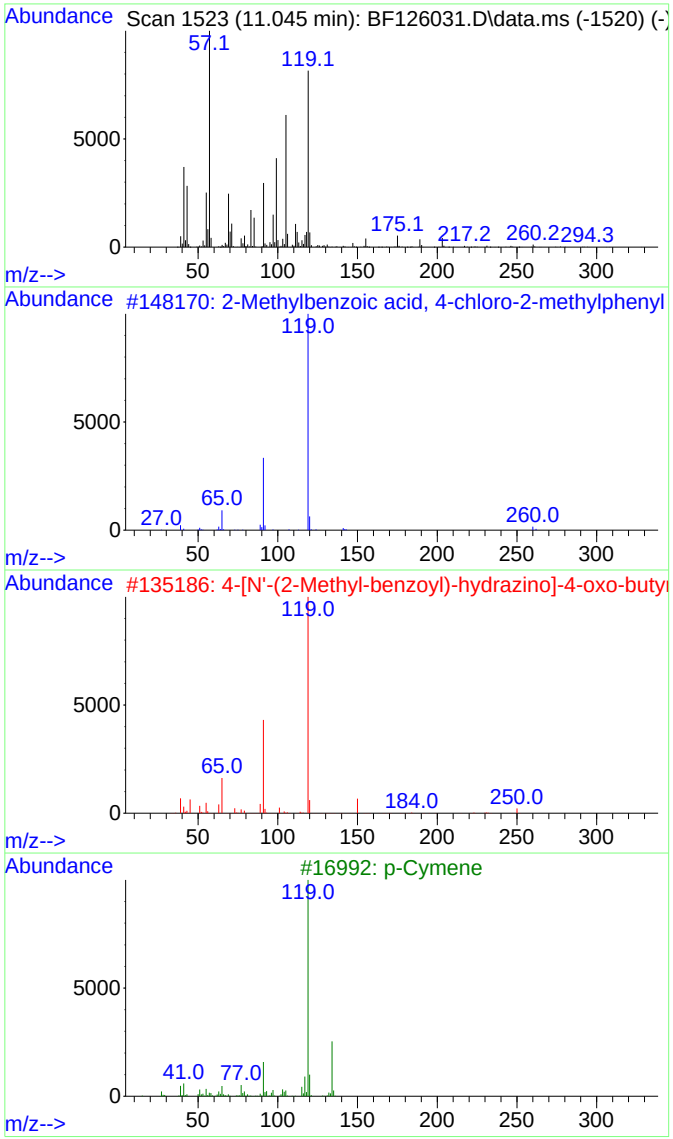
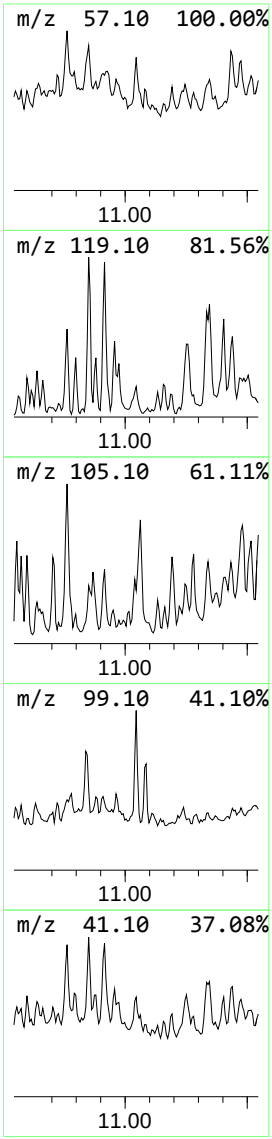
Peak Number 10 unknown11.045 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.045	41.73 ng	2240830	Phenanthrene-d10	11.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methylbenzoic acid, 4-chloro-2...	260	C15H13ClO2	1010331-28-1	27
2	4-[N'-(2-Methyl-benzoyl)-hydrazi...	250	C12H14N2O4	1000294-09-5	27
3	p-Cymene	134	C10H14	000099-87-6	27
4	(6-Chloro-2-methylhexan-2-yl)ben...	210	C13H19Cl	1417621-45-4	27
5	2-Hexanone, 5-methyl-5-phenyl-	190	C13H18O	014128-61-1	27





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TIC Library : C:\Database\NIST20.L
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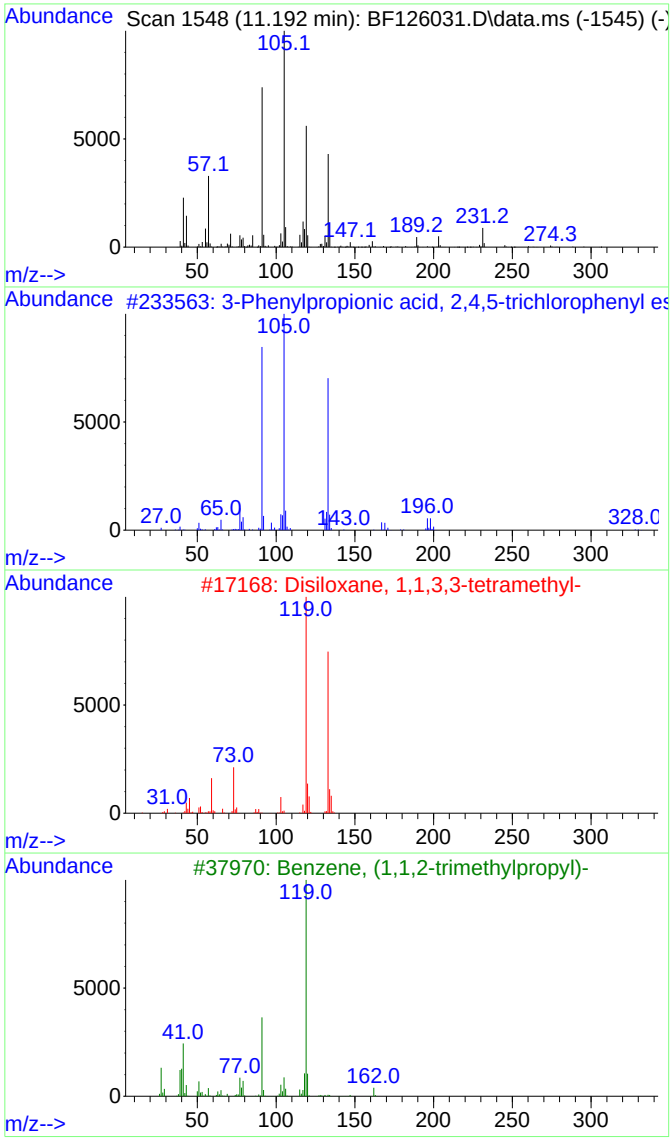
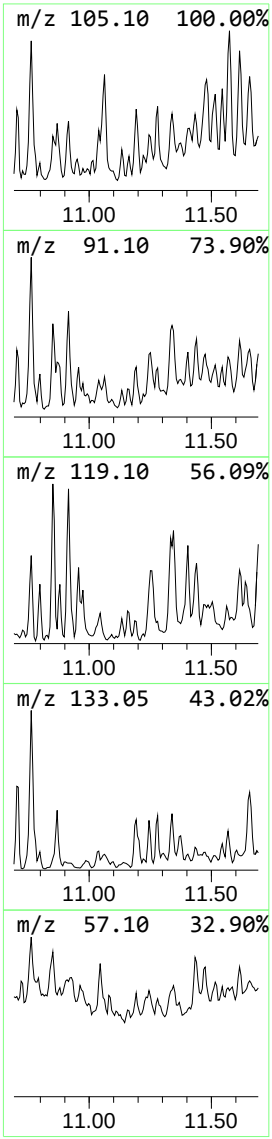
Peak Number 11 unknown11.192 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.192	42.59 ng	2286930	Phenanthrene-d10	11.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Phenylpropionic acid, 2,4,5-tr...	328	C15H11Cl3O2	1000354-74-5	43
2	Disiloxane, 1,1,3,3-tetramethyl-	134	C4H14OSi2	003277-26-7	43
3	Benzene, (1,1,2-trimethylpropyl)-	162	C12H18	026356-11-6	38
4	Diglycolic acid, 2-acetylphenyl ...	294	C15H18O6	1010382-71-7	35
5	Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	35





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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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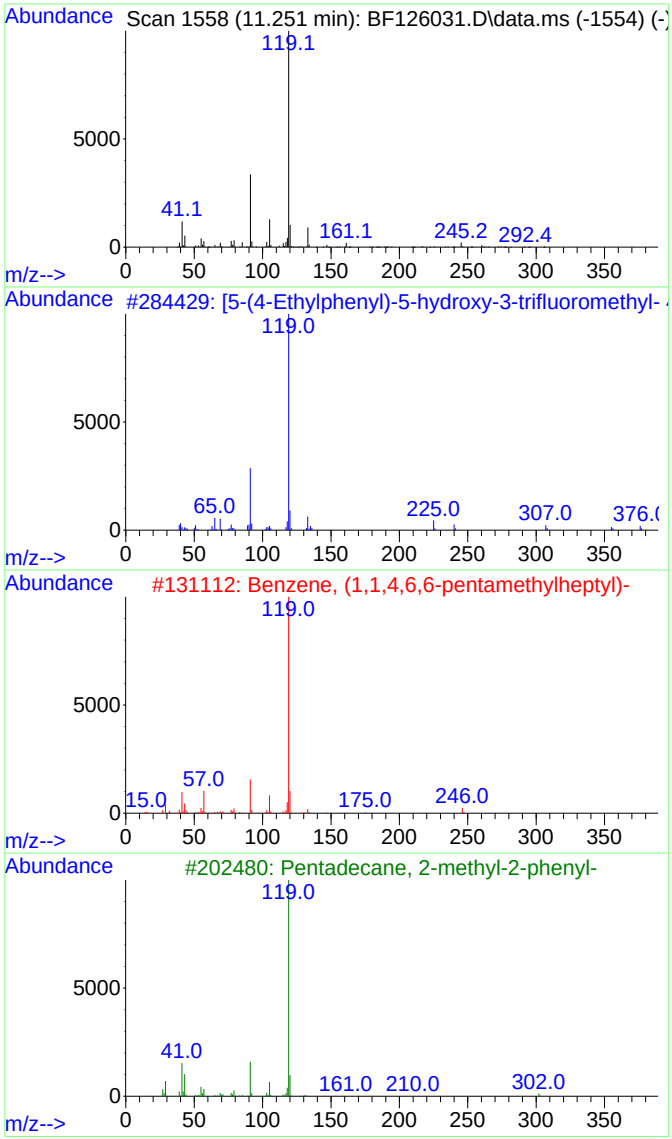
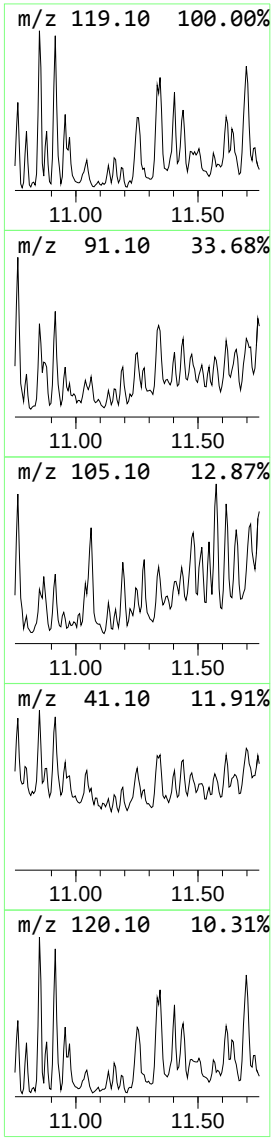
Peak Number 12 [5-(4-Ethylphenyl)-5-hydrox... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.251	77.25 ng	4148140	Phenanthrene-d10	11.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	[5-(4-Ethylphenyl)-5-hydroxy-3-t...	376	C20H19F3N2O2	1000311-59-5	72
2	Benzene, (1,1,4,6,6-pentamethylh...	246	C18H30	055134-07-1	72
3	Pentadecane, 2-methyl-2-phenyl-	302	C22H38	029138-94-1	64
4	Benzene, (1,1-dimethyldecyl)-	246	C18H30	027854-40-6	64
5	Dicumyl peroxide	270	C18H22O2	000080-43-3	64





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Misc :
ALS Vial : 18 Sample Multiplier: 1

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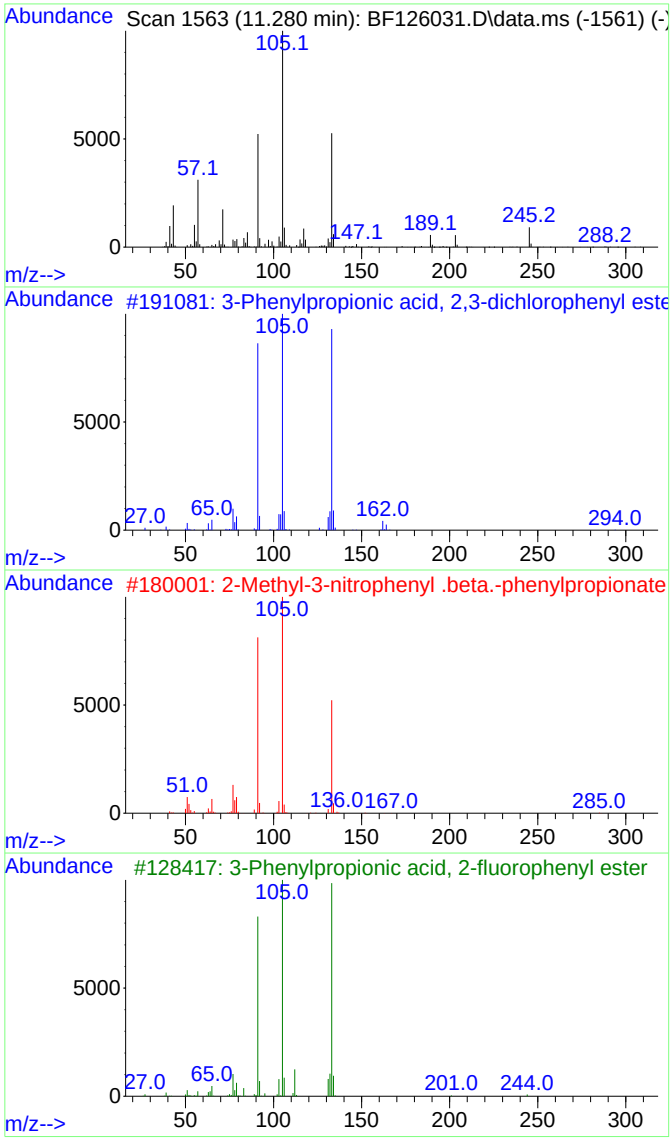
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

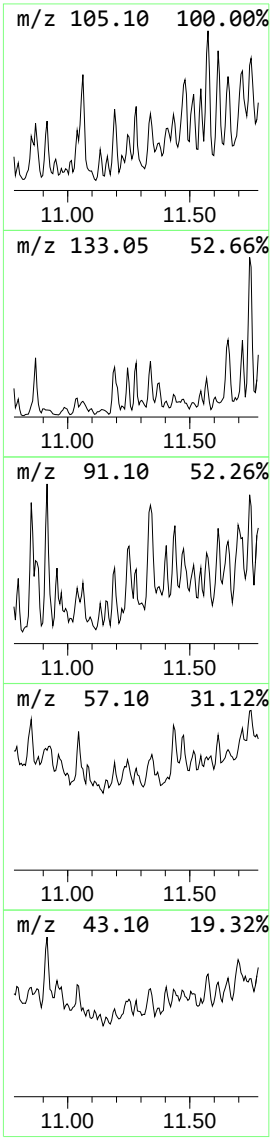
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 3-Phenylpropionic acid, 2,3... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.280	31.95 ng	1715930	Phenanthrene-d10	11.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Phenylpropionic acid, 2,3-dich...	294	C15H12Cl2O2	1000331-06-3	59
2	2-Methyl-3-nitrophenyl .beta.-ph...	285	C16H15NO4	040300-01-4	50
3	3-Phenylpropionic acid, 2-fluoro...	244	C15H13FO2	1000325-75-9	50
4	Undecanal, 3-phenyl-	246	C17H26O	147380-80-1	50
5	3-Phenylpropanoic acid, cyclobut...	204	C13H16O2	1000282-93-3	50





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Sample : M4427-08 5X
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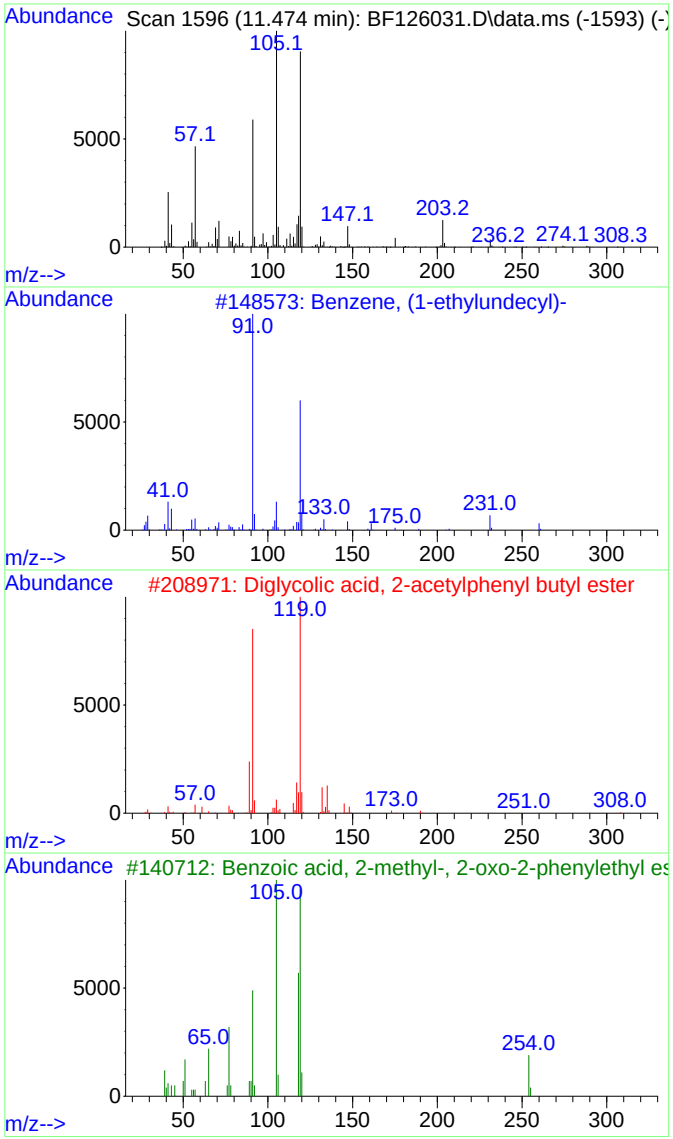
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

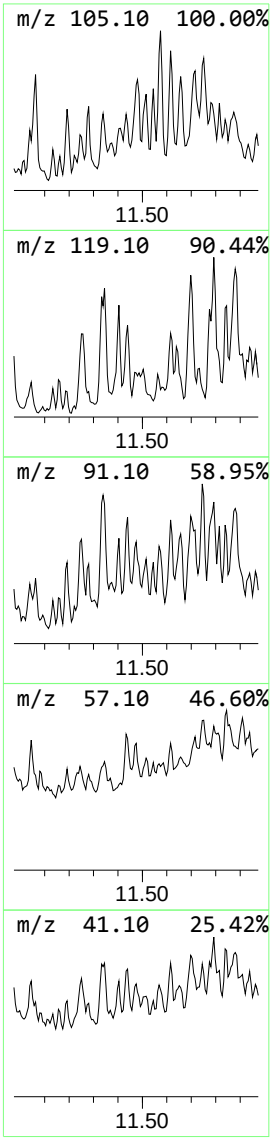
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 Diglycolic acid, 2-acetylph... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.474	49.48 ng	2657150	Phenanthrene-d10	11.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-ethylundecyl)-	260	C19H32	004534-52-5	59
2	Diglycolic acid, 2-acetylphenyl ...	308	C16H20O6	1000382-71-9	53
3	Benzoic acid, 2-methyl-, 2-oxo-2...	254	C16H14O3	055153-21-4	53
4	Diglycolic acid, 2-acetylphenyl ...	308	C16H20O6	1000382-71-8	50
5	Benzene, 1,1'-(1,1,2,2-tetrameth...	238	C18H22	001889-67-4	50





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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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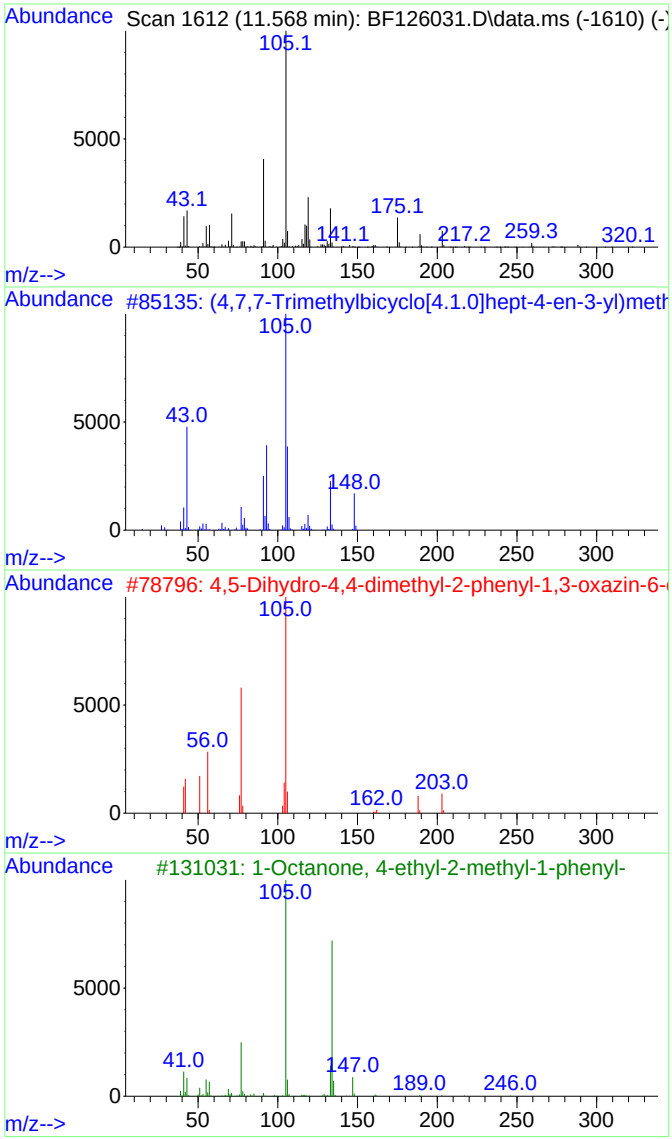
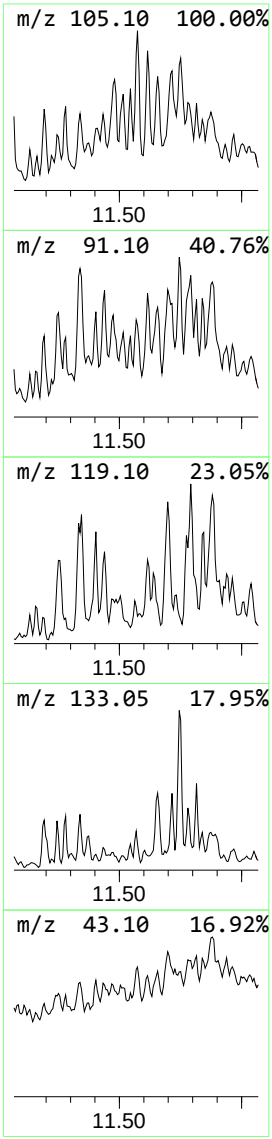
Peak Number 15 unknown11.568 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.568	59.41 ng	3190370	Phenanthrene-d10	11.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(4,7,7-Trimethylbicyclo[4.1.0]he...	208	C13H20O2	1000498-96-4	16
2	4,5-Dihydro-4,4-dimethyl-2-pheny...	203	C12H13NO2	029637-55-6	14
3	1-Octanone, 4-ethyl-2-methyl-1-p...	246	C17H26O	1914351-17-9	12
4	3-Phenylpropionic acid. 3,5-difl...	262	C15H12F2O2	1000299-02-0	10
5	2-Nitrophenyl-.beta.-phenylpropi...	271	C15H13NO4	040123-51-1	10





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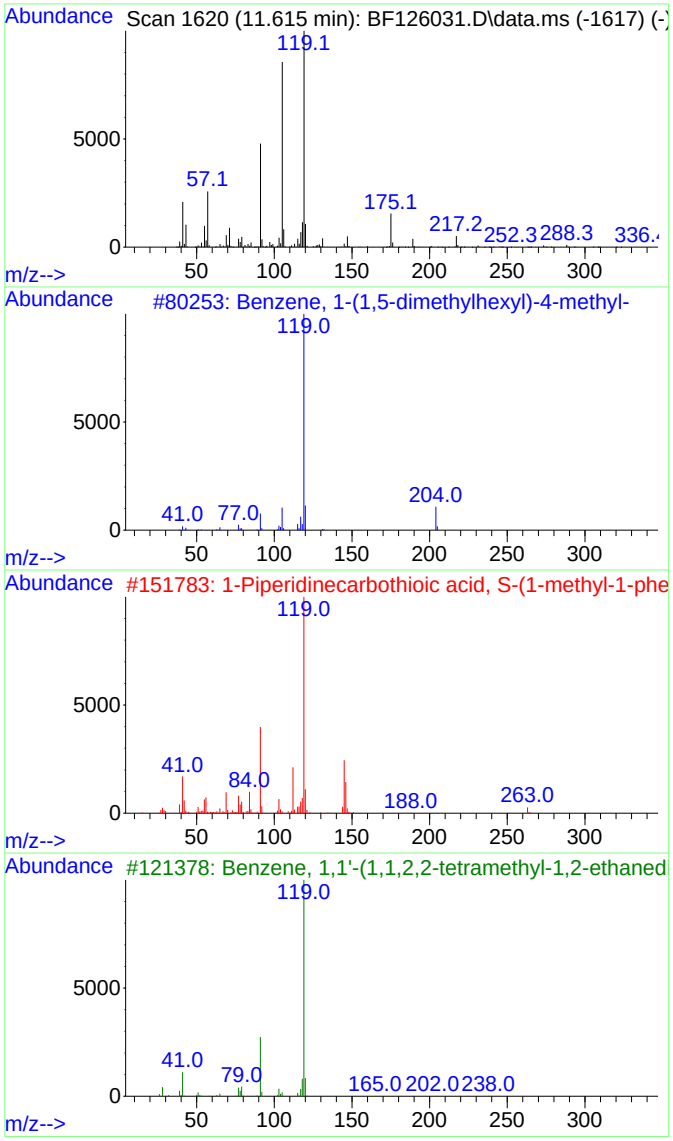
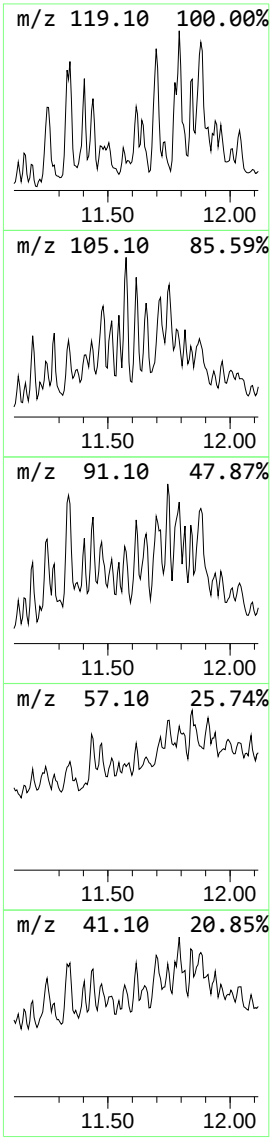
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 16 Benzene, 1-(1,5-dimethylhex... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	79.89 ng	4290250	Phenanthrene-d10	11.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-(1,5-dimethylhexyl)-4...	204	C15H24	001461-02-5	50
2	1-Piperidinecarbothioic acid, S-...	263	C15H21NOS	061432-55-1	50
3	Benzene, 1,1'-(1,1,2,2-tetrameth...	238	C18H22	001889-67-4	50
4	2-Hexanone, 5-methyl-5-phenyl-	190	C13H18O	014128-61-1	50
5	Ethanone, 2-bromo-1-(4-methylphe...	212	C9H9BrO	000619-41-0	50





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TIC Integration Parameters: LSCINT.P

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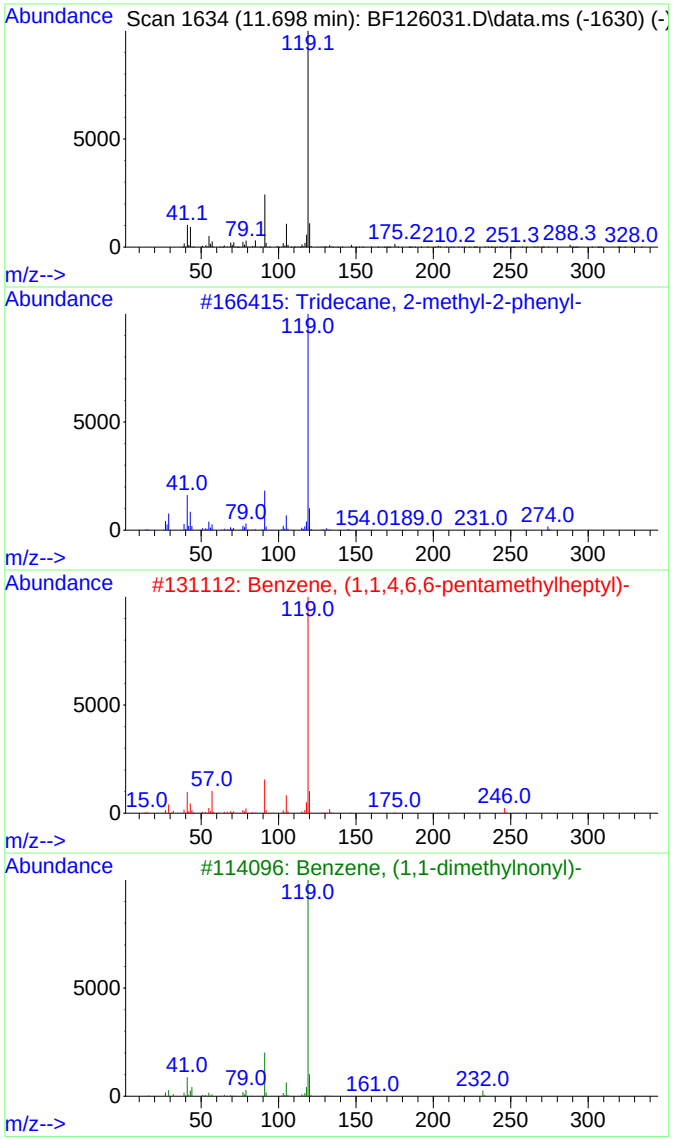
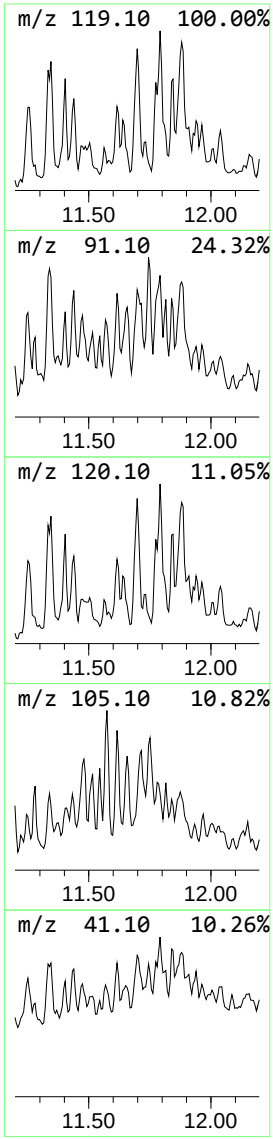
Peak Number 17 Tridecane, 2-methyl-2-phenyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.698	161.85 ng	8691170	Phenanthrene-d10	11.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 2-methyl-2-phenyl-	274	C20H34	027854-41-7	86
2	Benzene, (1,1,4,6,6-pentamethylh...	246	C18H30	055134-07-1	78
3	Benzene, (1,1-dimethylnonyl)-	232	C17H28	055191-25-8	78
4	Benzene, (1,1-dimethyldecyl)-	246	C18H30	027854-40-6	78
5	Pentadecane, 2-methyl-2-phenyl-	302	C22H38	029138-94-1	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110321\
Data File : BF126031.D
Acq On : 3 Nov 2021 21:27
Operator : JU/CG
Sample : M4427-08 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FDR-BH-2-20211029-6.5-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.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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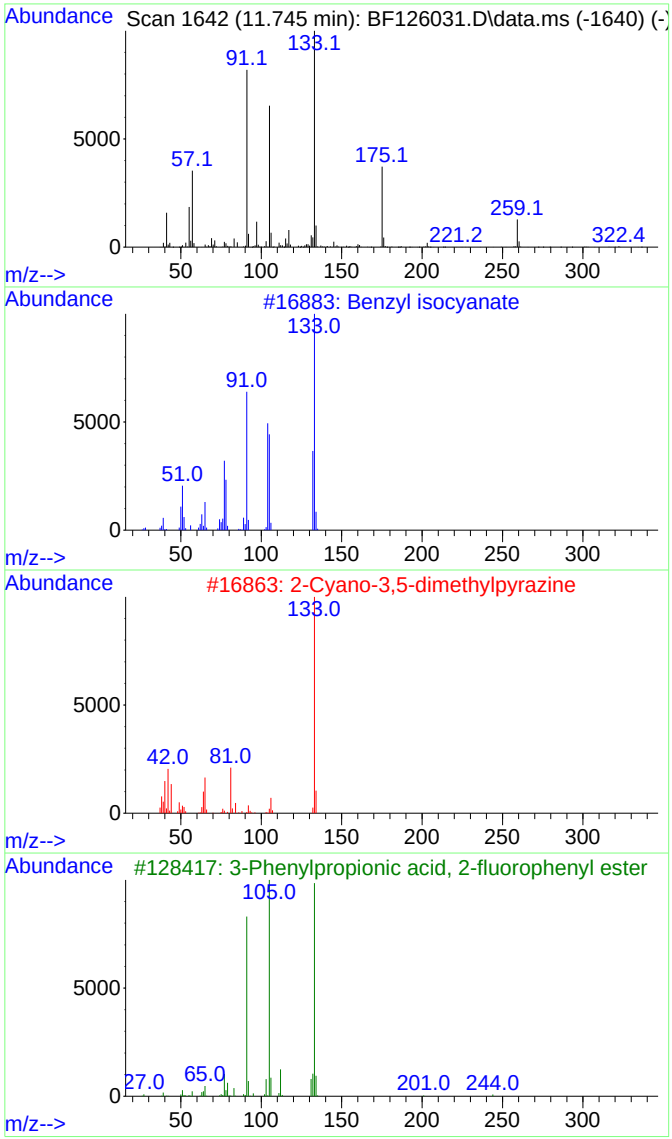
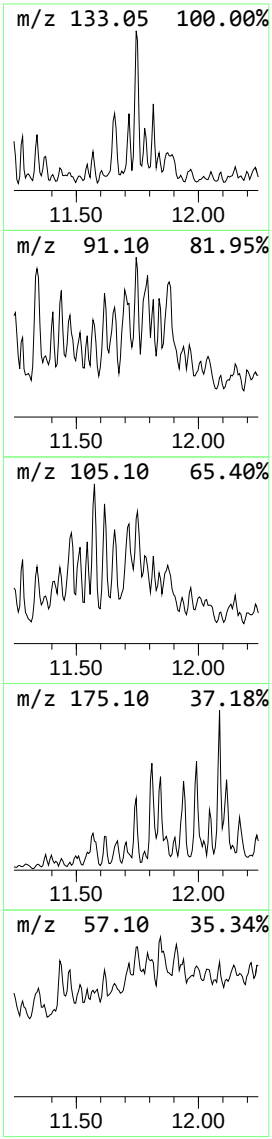
Peak Number 18 Benzyl isocyanate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.745	60.42 ng	3244290	Phenanthrene-d10	11.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzyl isocyanate	133	C8H7NO	003173-56-6	50
2	2-Cyano-3,5-dimethylpyrazine	133	C7H7N3	124629-52-3	43
3	3-Phenylpropionic acid, 2-fluoro...	244	C15H13FO2	1000325-75-9	40
4	3-Phenylpropionic acid, 4-cyanop...	251	C16H13NO2	1000307-78-4	40
5	1H-Indol-3-ol, acetate	175	C10H9NO2	000608-08-2	40





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110321\
Data File : BF126031.D
Acq On : 3 Nov 2021 21:27
Operator : JU/CG
Sample : M4427-08 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FDR-BH-2-20211029-6.5-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.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
Pentane, 2,2,4-...	8.898	44.9	ng	2690750	2	8.133	1198570	20.0
unknown9.410	9.410	37.5	ng	3231390	3	9.886	1722460	20.0
unknown10.386	10.386	29.3	ng	2520870	3	9.886	1722460	20.0
unknown10.433	10.433	50.8	ng	4372090	3	9.886	1722460	20.0
Benzene, 2-ethy...	10.763	162.7	ng	8738000	4	11.380	1073990	20.0
Benzene, (1,1-d...	10.798	37.1	ng	1993100	4	11.380	1073990	20.0
Benzene, (1,1,4...	10.851	103.0	ng	5533110	4	11.380	1073990	20.0
Cumene hydroper...	10.916	148.1	ng	7955010	4	11.380	1073990	20.0
Benzene, (1,1-d...	10.957	48.3	ng	2595810	4	11.380	1073990	20.0
unknown11.045	11.045	41.7	ng	2240830	4	11.380	1073990	20.0
unknown11.192	11.192	42.6	ng	2286930	4	11.380	1073990	20.0
[5-(4-Ethylphen...	11.251	77.3	ng	4148140	4	11.380	1073990	20.0
3-Phenylpropion...	11.280	31.9	ng	1715930	4	11.380	1073990	20.0
Diglycolic acid...	11.474	49.5	ng	2657150	4	11.380	1073990	20.0
unknown11.568	11.568	59.4	ng	3190370	4	11.380	1073990	20.0
Benzene, 1-(1,5...	11.616	79.9	ng	4290250	4	11.380	1073990	20.0
Tridecane, 2-me...	11.698	161.8	ng	8691170	4	11.380	1073990	20.0
Benzyl isocyanate	11.745	60.4	ng	3244290	4	11.380	1073990	20.0