LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083021\
Data File : BF125276.D
Acq On : 30 Aug 2021 22:37
Operator : JU/CG
Sample : M3561-17
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DAY-1

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-BF081821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125276.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	7	13	19	rBV	2096661	2676830	47.22%	2.049%
2	5.534	582	586	595	rBV	2368306	2107193	37.17%	1.613%
3	5.651	598	606	607	rBV2	77445	124729	2.20%	0.095%
4	5.675	607	610	612	rVV	116048	124893	2.20%	0.096%
5	5.704	612	615	622	rVB	401781	361697	6.38%	0.277%
6	5.810	628	633	635	rBV	182897	189857	3.35%	0.145%
7	5.963	653	659	663	rBV	230504	206988	3.65%	0.158%
8	6.239	701	706	714	rBV4	103043	173612	3.06%	0.133%
9	6.316	714	719	721	rBV	127519	134087	2.37%	0.103%
10	6.416	733	736	742	rVB	201398	189791	3.35%	0.145%
11	6.545	754	758	762	rVB	1469132	1312130	23.15%	1.004%
12	6.616	762	770	773	rVB2	101312	136961	2.42%	0.105%
13	6.792	797	800	805	rBV3	165612	202592	3.57%	0.155%
14	6.839	805	808	810	rBV	138369	131409	2.32%	0.101%
15	6.916	817	821	825	rBV2	1523571	1453087	25.63%	1.112%
16	6.992	832	834	840	rVB	134149	132965	2.35%	0.102%
17	7.063	840	846	848	rBV	288180	322460	5.69%	0.247%
18	7.092	848	851	854	rVV3	230825	289876	5.11%	0.222%
19	7.134	854	858	860	rVV3	152678	194472	3.43%	0.149%
20	7.239	872	876	879	rBV4	118210	211095	3.72%	0.162%
21	7.351	885	895	897	rBV	483366	949384	16.75%	0.727%
22	7.445	905	911	913	rBV	505983	634049	11.19%	0.485%
23	7.481	913	917	920	rVV	3407188	2843255	50.16%	2.176%
24	7.557	927	930	935	rBV5	178388	315589	5.57%	0.242%
25	7.598	935	937	940	rVV2	331515	302931	5.34%	0.232%
26	7.628	940	942	944	rVV	197593	203294	3.59%	0.156%
27	7.681	948	951	955	rVB3	683224	665730	11.74%	0.510%
28	7.722	955	958	962	rBV4	100099	171176	3.02%	0.131%
29	7.804	968	972	975	rBV2	184251	261644	4.62%	0.200%
30	7.863	975	982	985	rVV3	931302	1641064	28.95%	1.256%
31	7.910	985	990	992	rBV3	191766	213880	3.77%	0.164%
32	7.933	992	994	998	rVV2	564759	552949	9.75%	0.423%
33	7.986	999	1003	1006	rVV2	631229	699441	12.34%	0.535%
34	8.016	1006	1008	1013	rVB4	460676	729759	12.87%	0.559%
35	8.063	1013	1016	1018	rBV2	177558	165156	2.91%	0.126%
36	8.175	1025	1035	1036	rBV4	974733	2405395	42.43%	1.841%

LSC Area Percent Report

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Instrument : BNA_F
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Integration Parameters: rteint.p
Integrator: RTE
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Sampling : 1 Min Area: 3 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	8.198	1036	1039	1041	rVV	1538112	1538080	27.13%	1.177%
38	8.245	1045	1047	1051	rVB3	512401	624569	11.02%	0.478%
39	8.281	1051	1053	1055	rVB	381830	257959	4.55%	0.197%
40	8.351	1055	1065	1068	rBV3	1006896	1677049	29.58%	1.284%
41	8.392	1068	1072	1074	rBV4	387391	538078	9.49%	0.412%
42	8.445	1077	1081	1084	rBV3	810545	974140	17.18%	0.746%
43	8.475	1084	1086	1089	rVB3	645284	574549	10.14%	0.440%
44	8.510	1089	1092	1098	rBV4	314773	531230	9.37%	0.407%
45	8.581	1098	1104	1105	rBV3	768833	1003762	17.71%	0.768%
46	8.610	1105	1109	1112	rVB2	1216953	1453399	25.64%	1.112%
47	8.663	1112	1118	1123	rBV5	1236478	1989225	35.09%	1.523%
48	8.704	1123	1125	1128	rVB2	863111	809886	14.29%	0.620%
49	8.745	1128	1132	1136	rVB4	780098	956614	16.88%	0.732%
50	8.798	1136	1141	1144	rBV4	1070009	1926891	33.99%	1.475%
51	8.828	1144	1146	1147	rBV	271745	187640	3.31%	0.144%
52	8.851	1147	1150	1154	rVB5	486027	735329	12.97%	0.563%
53	8.904	1154	1159	1163	rVB3	1119858	2063972	36.41%	1.580%
54	8.945	1163	1166	1168	rBV3	868413	1075026	18.96%	0.823%
55	9.010	1171	1177	1183	rBV2	3181271	4902034	86.47%	3.752%
56	9.069	1183	1187	1190	rVB4	1115635	1672800	29.51%	1.280%
57	9.110	1190	1194	1197	rBV4	844513	1307129	23.06%	1.000%
58	9.145	1197	1200	1206	rBV2	865179	1589214	28.03%	1.216%
59	9.204	1206	1210	1212	rVB3	1245653	1338222	23.61%	1.024%
60	9.233	1212	1215	1218	rBV4	652551	942422	16.62%	0.721%
61	9.275	1218	1222	1225	rVB	5359169	4407876	77.76%	3.374%
62	9.298	1225	1226	1227	rVB	391224	138102	2.44%	0.106%
63	9.328	1227	1231	1235	rVB5	805290	947407	16.71%	0.725%
64	9.369	1236	1238	1240	rBV	365754	261974	4.62%	0.201%
65	9.398	1240	1243	1244	rBV	644180	583456	10.29%	0.447%
66	9.445	1249	1251	1254	rBV	1508042	1693725	29.88%	1.296%
67	9.545	1263	1268	1271	rBV2	2485708	3854578	68.00%	2.950%
68	9.616	1276	1280	1283	rBV2	3039991	5164116	91.10%	3.953%
69	9.675	1287	1290	1292	rBV2	855501	1014138	17.89%	0.776%
70	9.698	1292	1294	1298	rVV3	782977	821661	14.49%	0.629%
71	9.816	1309	1314	1316	rBV3	666267	1035458	18.27%	0.793%
72	9.869	1319	1323	1325	rVV2	1809690	2010098	35.46%	1.539%
73	9.922	1329	1332	1334	rVB	1409226	1228523	21.67%	0.940%
74	9.963	1334	1339	1346	rBV5	3145320	5668737	100.00%	4.339%
75	10.016	1346	1348	1351	rBV3	1097882	1205714	21.27%	0.923%
76	10.051	1351	1354	1357	rVV2	2383575	2167750	38.24%	1.659%

LSC Area Percent Report

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	10.133	1361	1368	1371	rBV4	2942151	4792070	84.54%	3.668%
78	10.163	1371	1373	1376	rVB3	1187789	1119429	19.75%	0.857%
79	10.233	1383	1385	1387	rBV2	471148	382895	6.75%	0.293%
80	10.275	1387	1392	1393	rBV2	1496869	1771202	31.25%	1.356%
81	10.292	1393	1395	1399	rVB2	1643391	1528261	26.96%	1.170%
82	10.333	1399	1402	1406	rBV5	944317	1876827	33.11%	1.436%
83	10.404	1412	1414	1416	rVB	1544883	1237772	21.84%	0.947%
84	10.510	1430	1432	1434	rVB	930321	605057	10.67%	0.463%
85	10.533	1434	1436	1441	rVB4	1445267	1666136	29.39%	1.275%
86	10.592	1441	1446	1447	rBV4	1848465	2782751	49.09%	2.130%
87	10.710	1463	1466	1470	rBV6	1152612	1619991	28.58%	1.240%
88	10.763	1470	1475	1477	rBV3	3160514	3897034	68.75%	2.983%
89	10.892	1494	1497	1499	rVB2	1175573	1182086	20.85%	0.905%
90	10.974	1508	1511	1515	rVB4	1809508	2058886	36.32%	1.576%
91	11.457	1590	1593	1602	rVB3	1657295	3188339	56.24%	2.440%
92	11.533	1603	1606	1608	rVV	934307	1220254	21.53%	0.934%
93	11.580	1611	1614	1619	rVB	2719752	2893489	51.04%	2.215%
94	11.727	1636	1639	1643	rBV2	933174	959879	16.93%	0.735%
95	11.874	1661	1664	1666	rBV2	939721	1030589	18.18%	0.789%
96	11.904	1666	1669	1675	rVB2	1382563	2285085	40.31%	1.749%
97	12.786	1817	1819	1825	rVB6	703054	847806	14.96%	0.649%
98	13.045	1859	1863	1865	rVB	3395080	3188524	56.25%	2.440%
99	14.104	2040	2043	2047	rVB	1111473	1185058	20.91%	0.907%
100	15.604	2293	2298	2302	rVB	814159	1029607	18.16%	0.788%

Sum of corrected areas: 130652979

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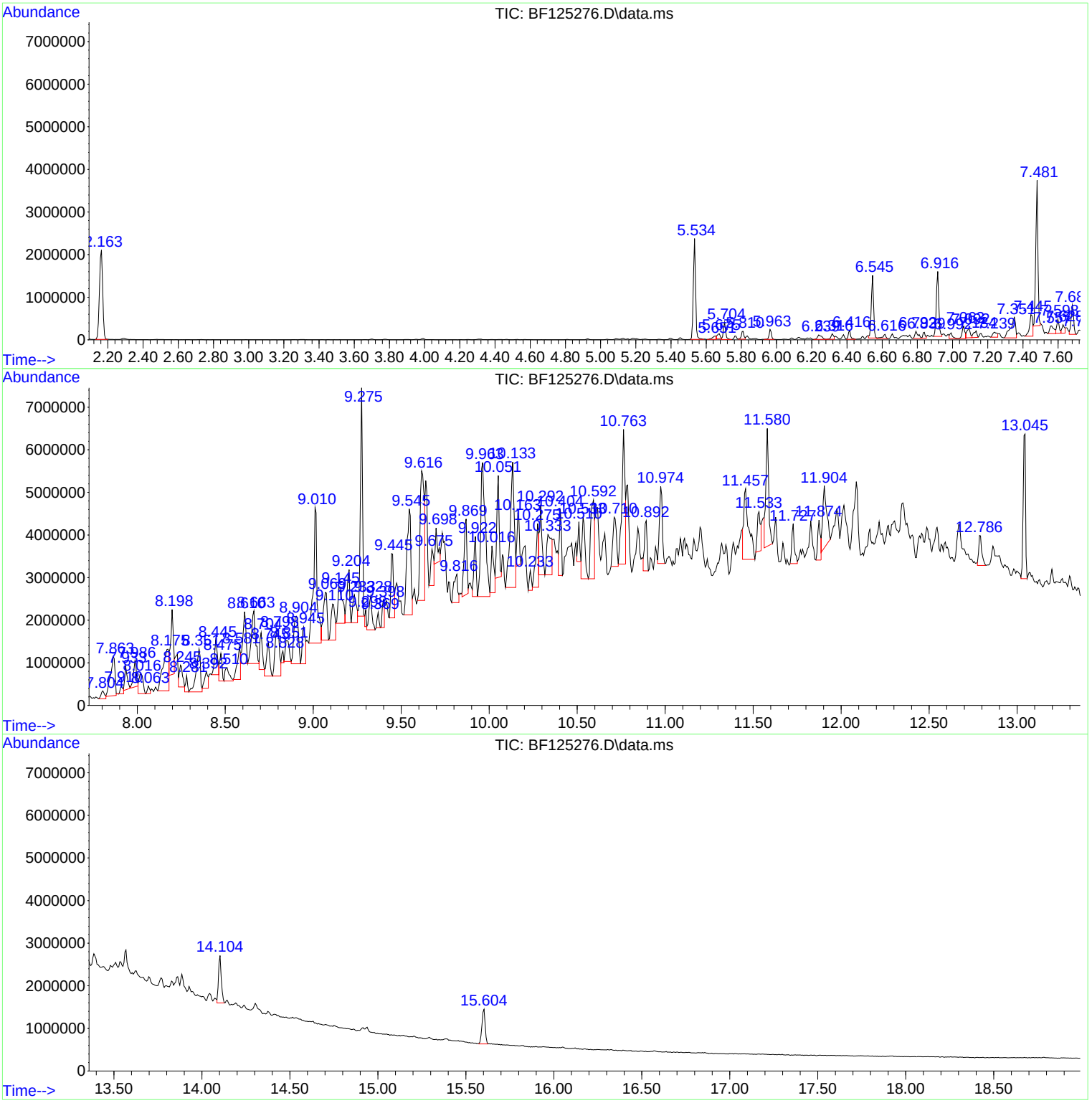
Instrument :
BNA_F
ClientSampleId :
DAY-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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\BF083021\
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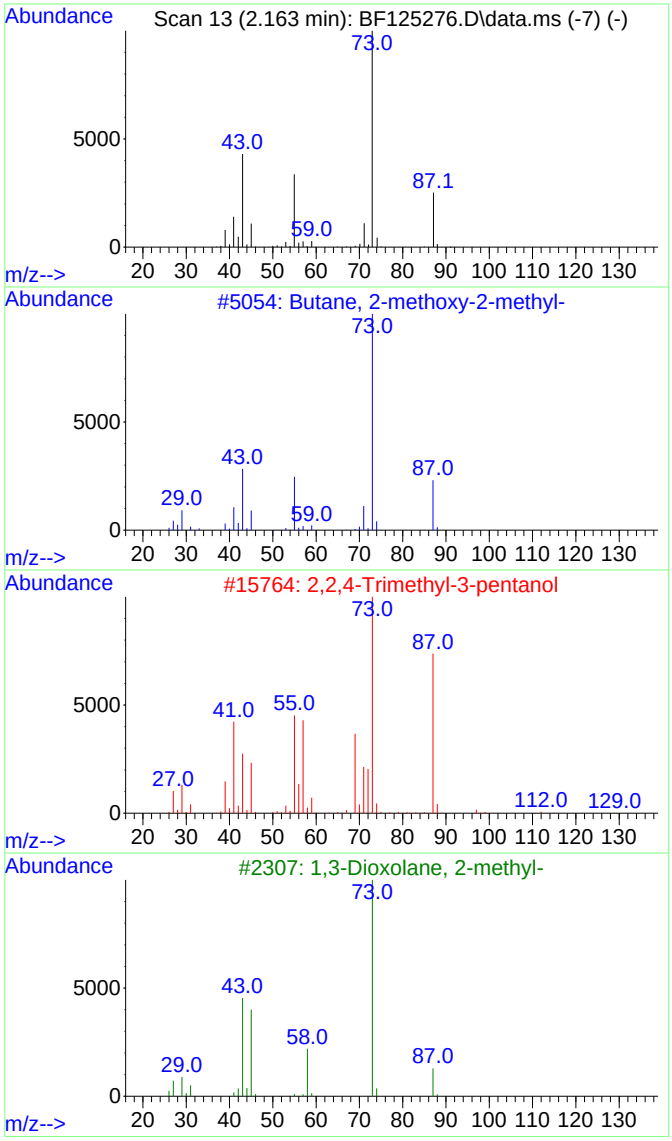
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

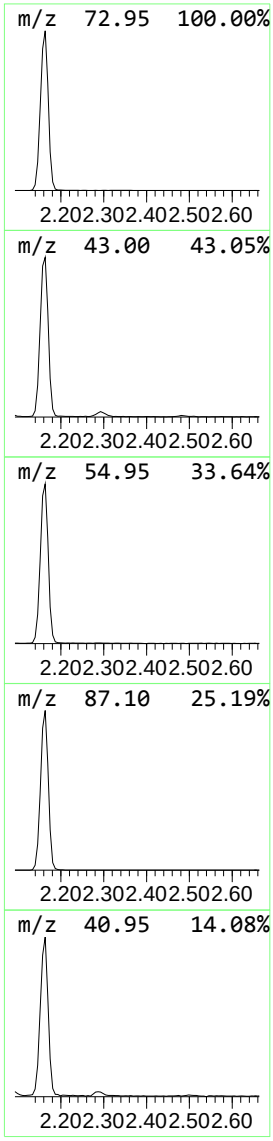
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.163	36.84 ng	2676830	1,4-Dichlorobenzene-d4	6.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

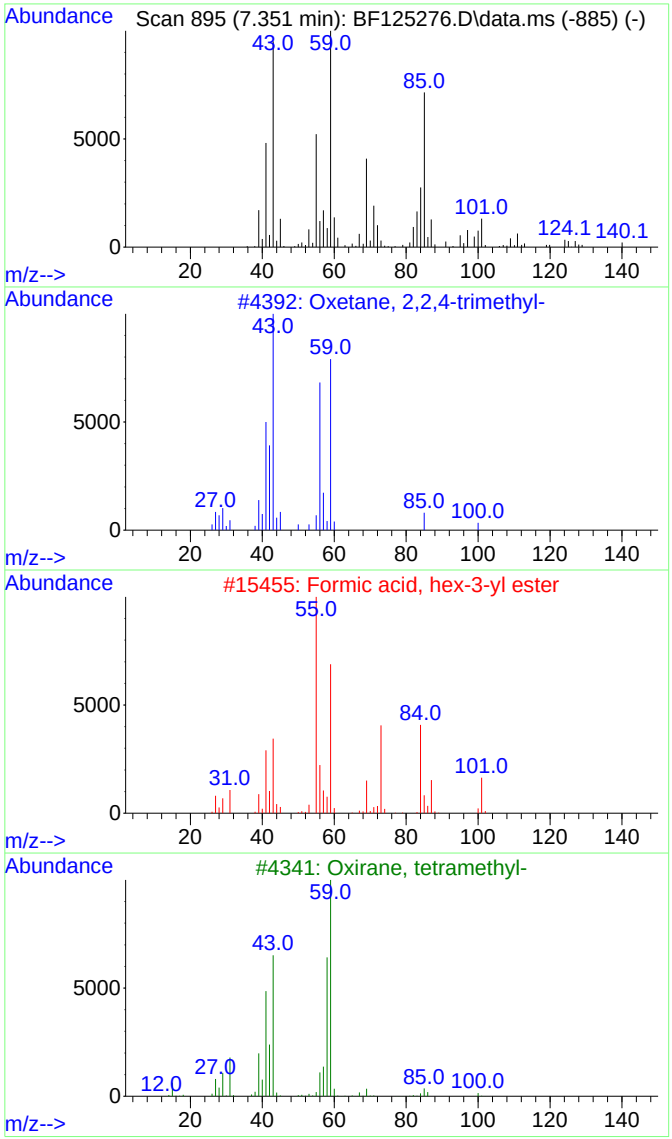
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

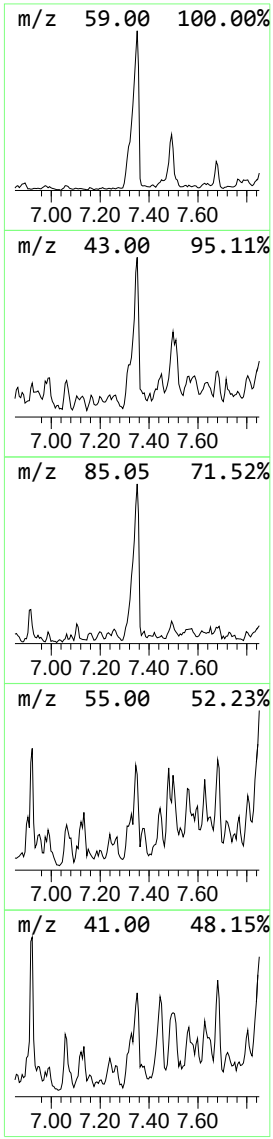
****

Peak Number 2 unknown7.351 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.351	13.07 ng	949384	1,4-Dichlorobenzene-d4	6.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxetane, 2,2,4-trimethyl-	100	C6H12O	023120-44-7	47
2	Formic acid, hex-3-yl ester	130	C7H14O2	1000367-94-4	27
3	Oxirane, tetramethyl-	100	C6H12O	005076-20-0	27
4	5-Hydroxypentanal acetate	144	C7H12O3	018545-16-9	14
5	Allyldimethylsilane	100	C5H12Si	003937-30-2	14





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

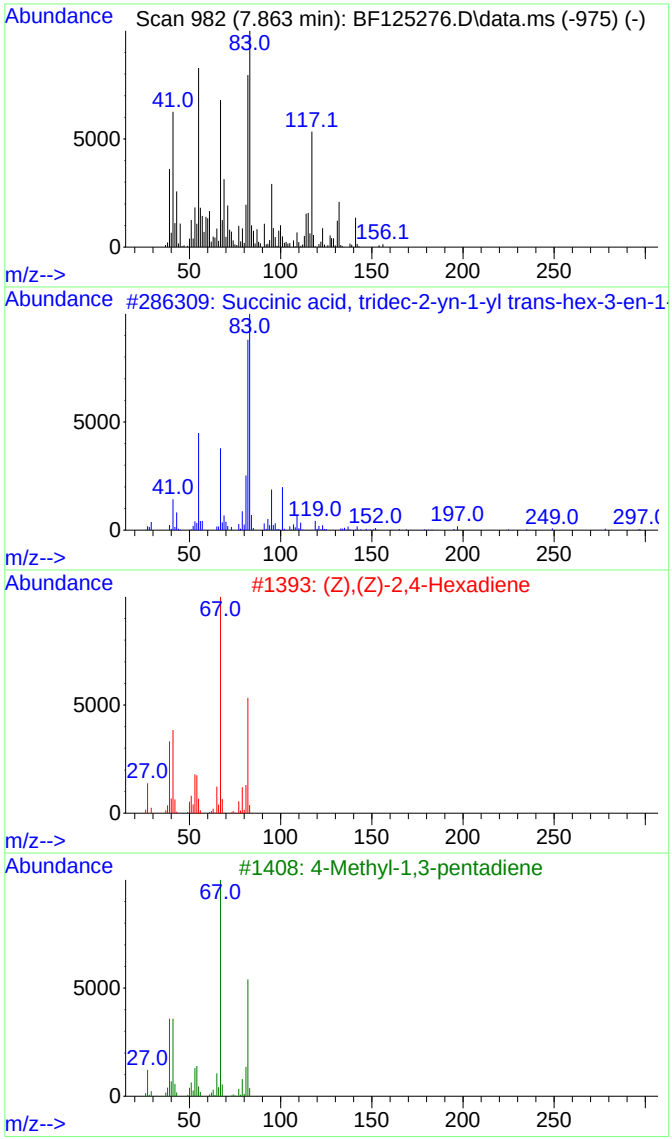
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

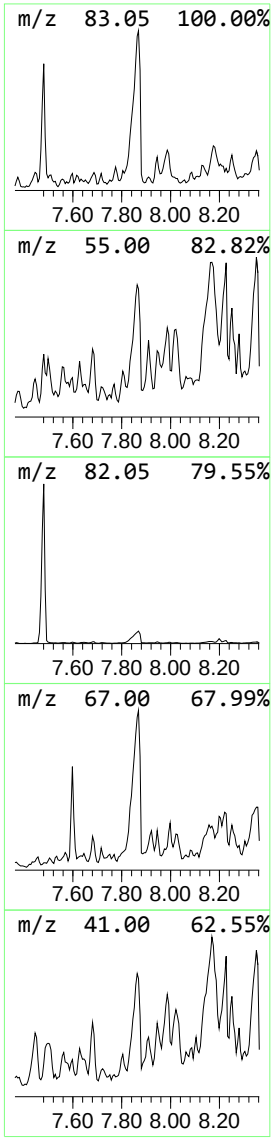
****

Peak Number 3 unknown7.863 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.863	21.34 ng	1641060	Naphthalene-d8	8.198

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Succinic acid, tridec-2-yn-1-yl ...	378	C23H38O4	1000391-12-6	47
2	(Z),(Z)-2,4-Hexadiene	82	C6H10	006108-61-8	30
3	4-Methyl-1,3-pentadiene	82	C6H10	000926-56-7	30
4	2-Hexyne	82	C6H10	000764-35-2	30
5	2,4-Hexadiene, (E,E)-	82	C6H10	005194-51-4	30





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Instrument : BNA_F
ClientSampleId : DAY-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

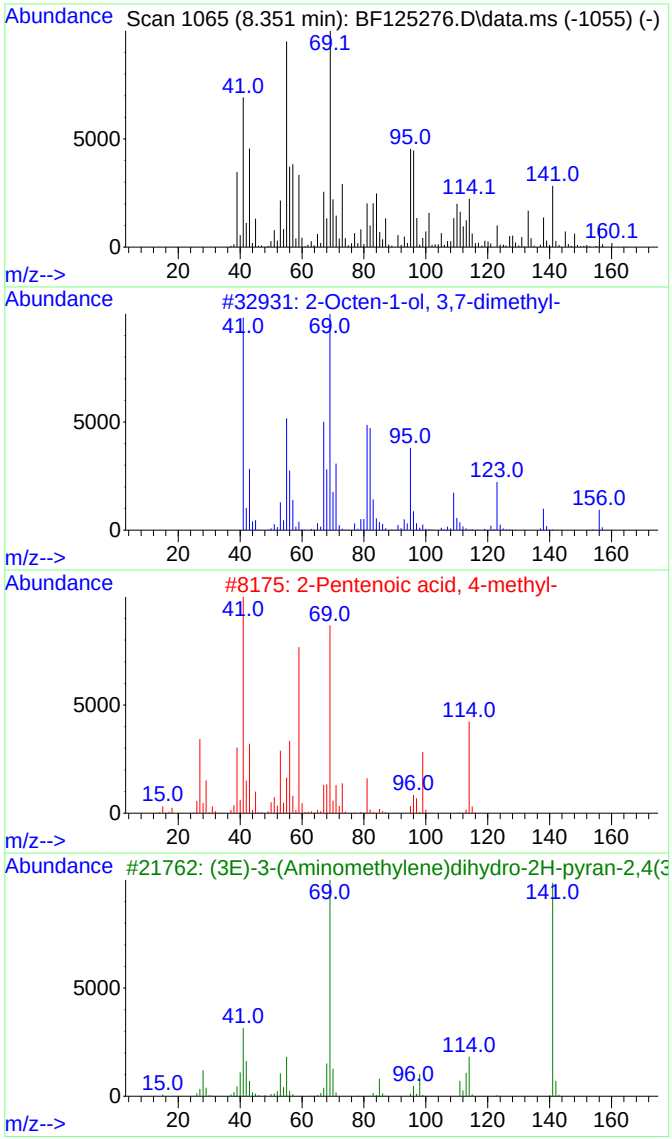
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

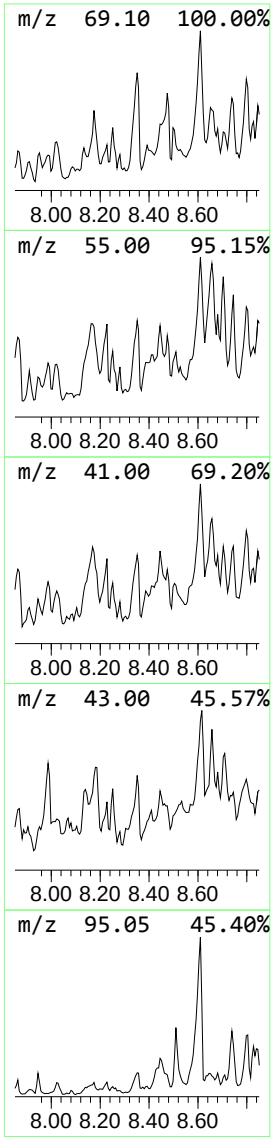
****

Peak Number 4 unknown8.351 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.351	21.81 ng	1677050	Naphthalene-d8	8.198

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octen-1-ol, 3,7-dimethyl-	156	C10H20O	040607-48-5	35
2	2-Pentenoic acid, 4-methyl-	114	C6H10O2	010321-71-8	30
3	(3E)-3-(Aminomethylene)dihydro-2...	141	C6H7NO3	022108-77-6	27
4	2-Pentenoic acid, 2-methyl-	114	C6H10O2	003142-72-1	27
5	Pentane, 3-methylene-	84	C6H12	000760-21-4	25





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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DAY-1

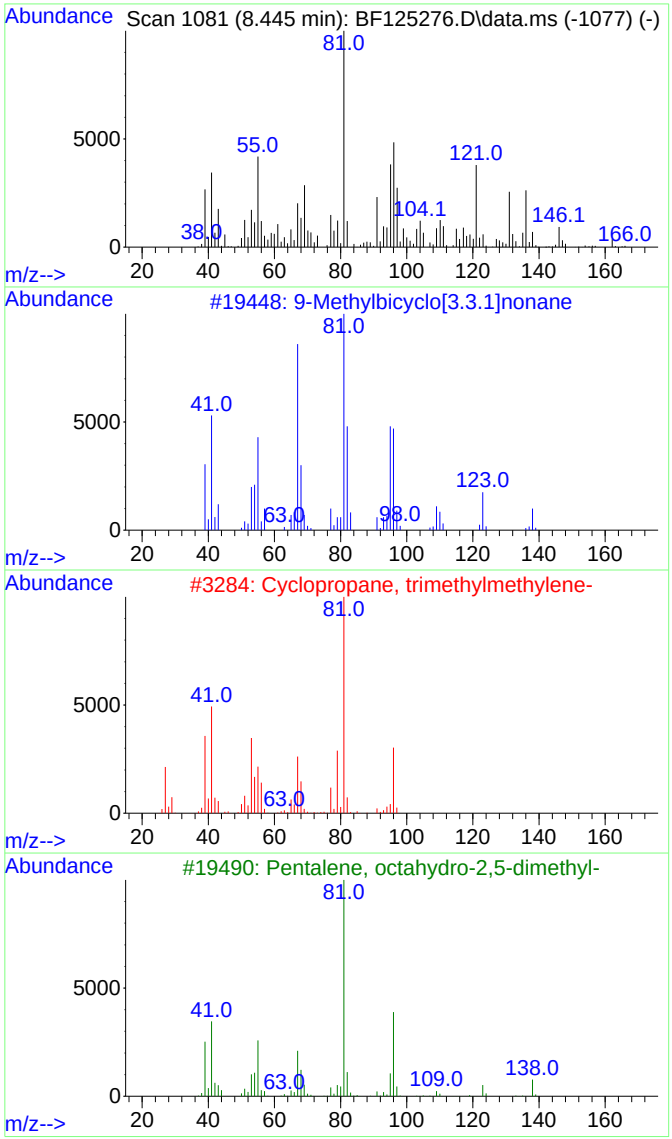
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

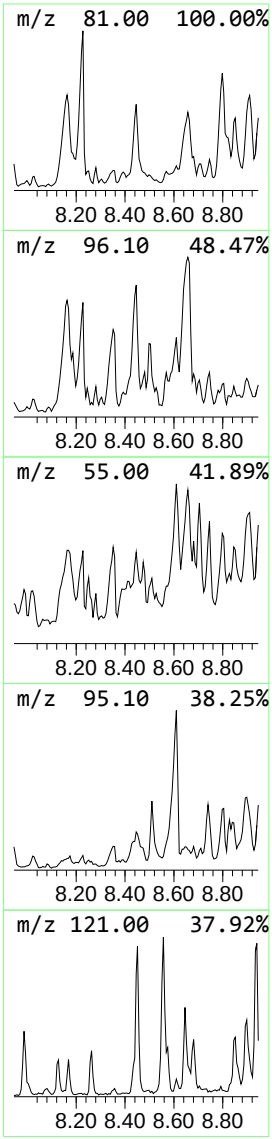
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 9-Methylbicyclo[3.3.1]nonane Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.445	12.67 ng	974140	Naphthalene-d8	8.198

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Methylbicyclo[3.3.1]nonane	138	C10H18	025107-01-1	58
2	Cyclopropane, trimethylmethylene-	96	C7H12	034462-28-7	45
3	Pentalene, octahydro-2,5-dimethyl-	138	C10H18	028588-55-8	45
4	Cyclohexene, 1-methyl-	96	C7H12	000591-49-1	43
5	trans-4-Methylcyclohexanol, trif...	210	C9H13F3O2	1000364-13-8	43





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Acq On : 30 Aug 2021 22:37
Operator : JU/CG
Sample : M3561-17
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DAY-1

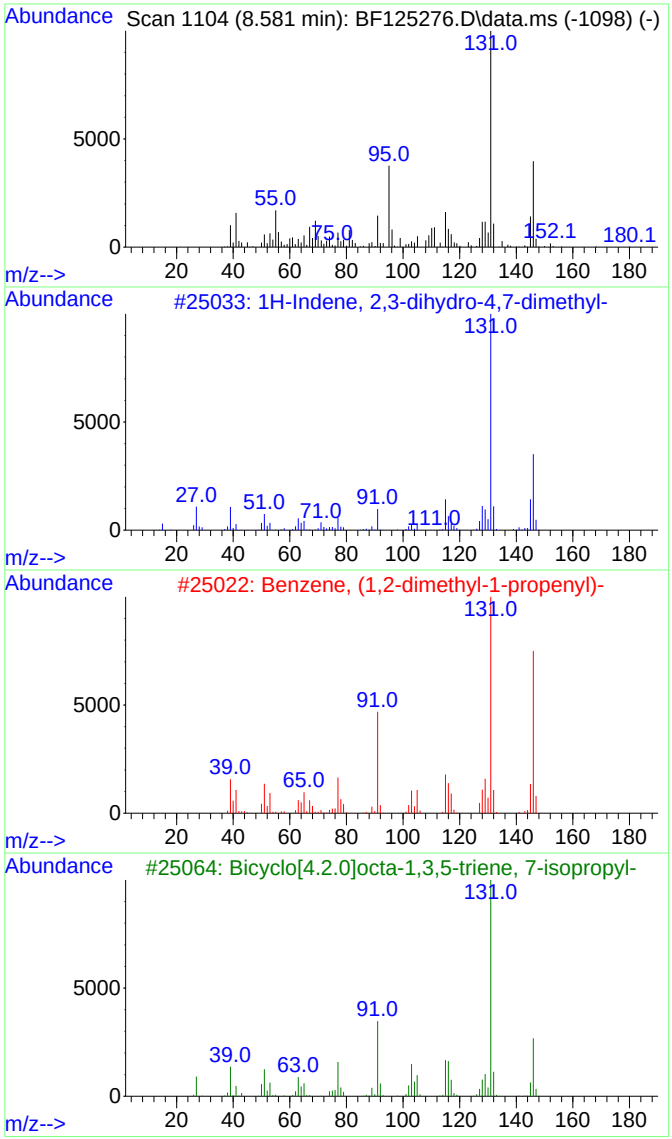
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

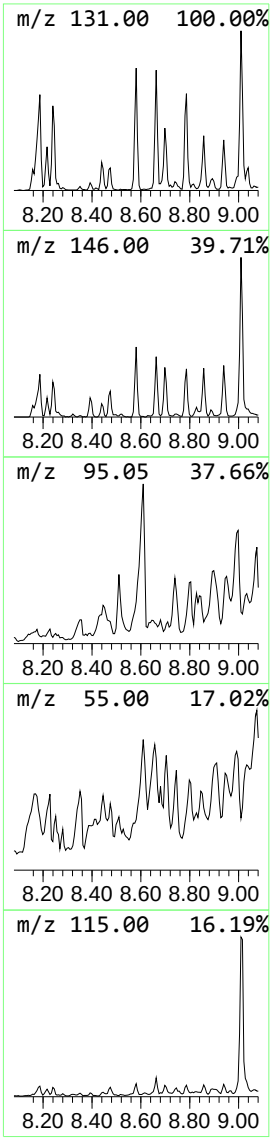
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1H-Indene, 2,3-dihydro-4,7-... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.581	13.05 ng	1003760	Naphthalene-d8	8.198

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	95
2	Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	94
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	146	C11H14	027087-54-3	90
4	Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	90
5	1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	87





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Operator : JU/CG
Sample : M3561-17
Misc :
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Instrument : BNA_F
ClientSampleId : DAY-1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

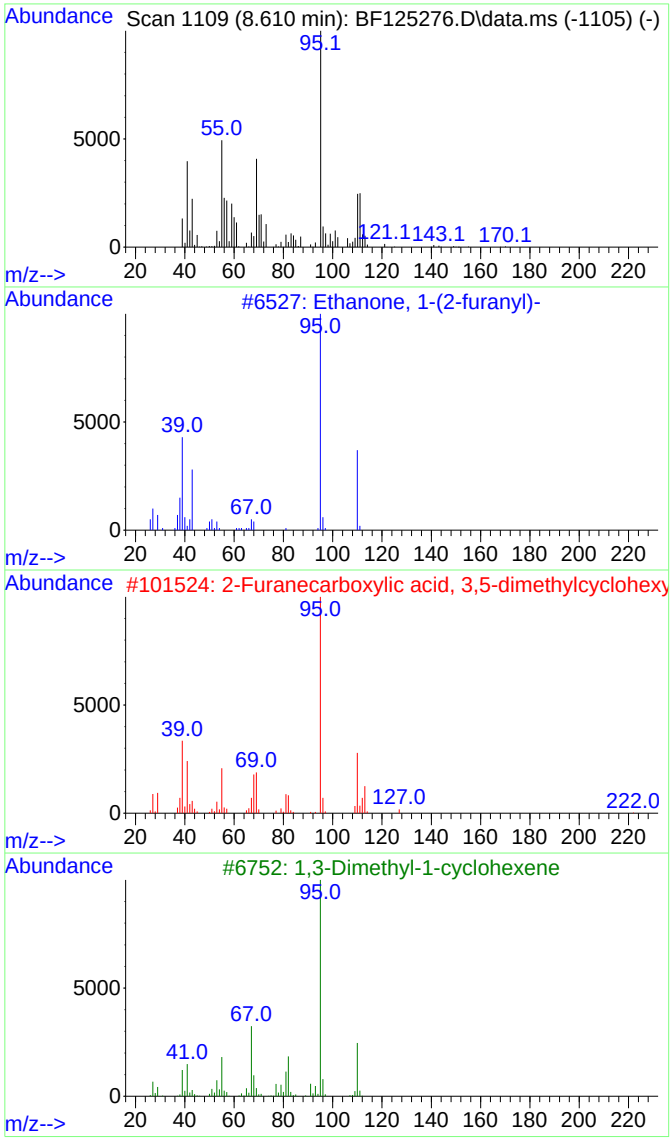
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

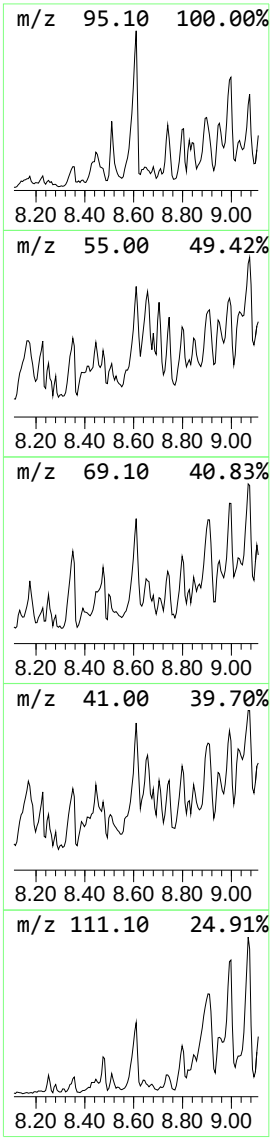
****

Peak Number 7 unknown8.610 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.610	18.90 ng	1453400	Naphthalene-d8	8.198

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanone, 1-(2-furanyl)-	110	C6H6O2	001192-62-7	46
2	2-Furanecarboxylic acid, 3,5-dim...	222	C13H18O3	1000278-87-2	43
3	1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	43
4	2-Furanecarboxylic acid, 2-butyl...	168	C9H12O3	116668-42-9	38
5	1,3-Dimethyl-5-heptafluorobutyry...	324	C12H15F7O2	1000216-63-8	38





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Sample : M3561-17
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DAY-1

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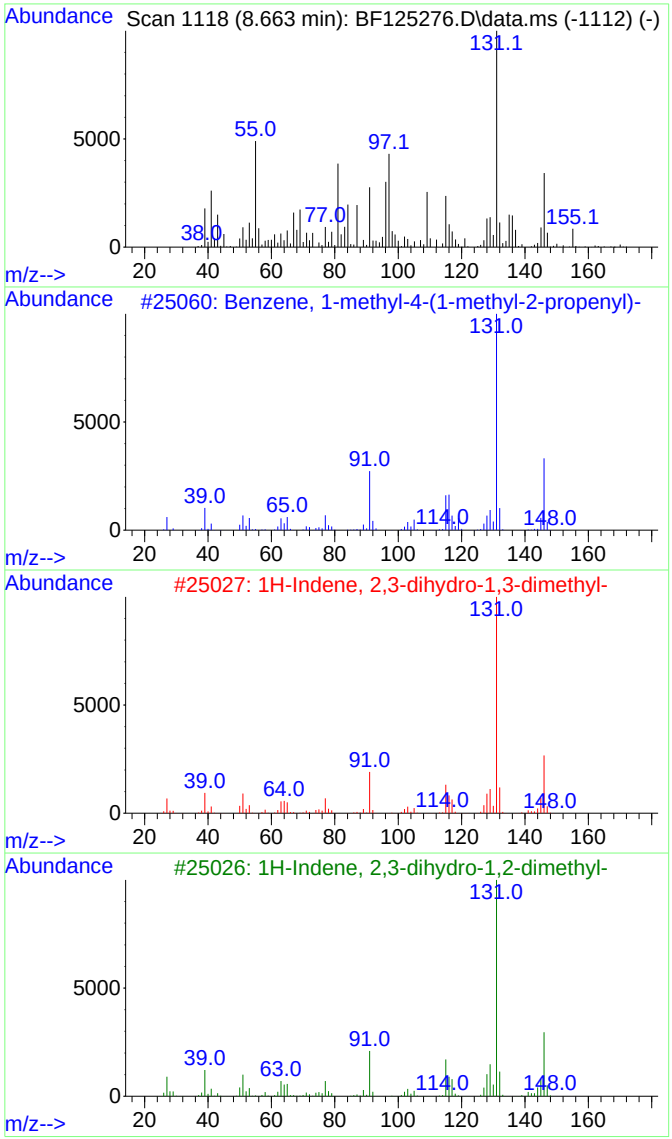
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

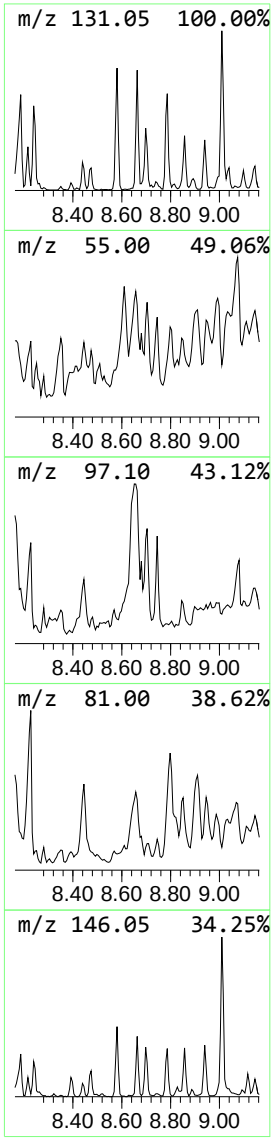
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1-methyl-4-(1-meth... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.663	25.87 ng	1989230	Naphthalene-d8	8.198

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-4-(1-methyl-2-...	146	C11H14	097664-18-1	55
2	1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	55
3	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	55
4	Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	42
5	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	42





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Sample : M3561-17
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DAY-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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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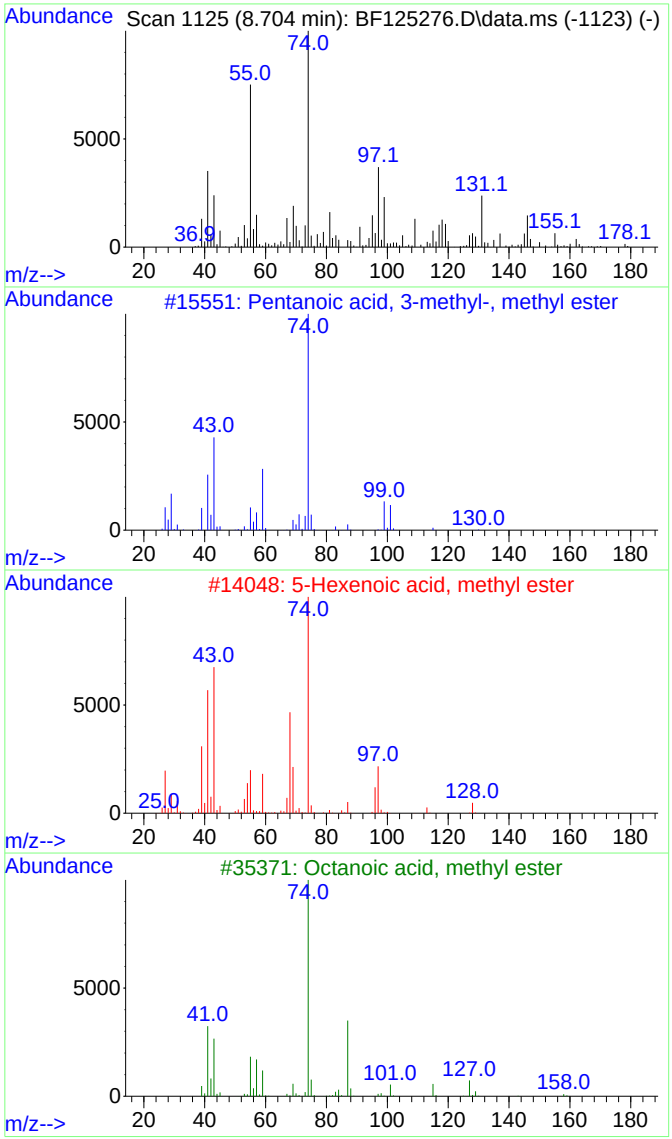
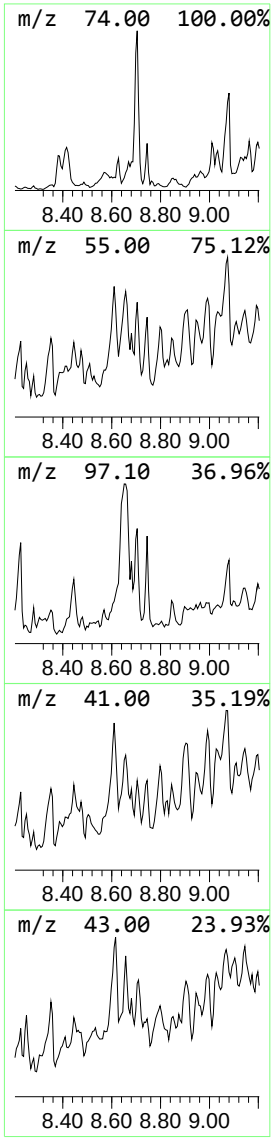
Peak Number 9 unknown8.704 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.704	10.53 ng	809886	Naphthalene-d8	8.198

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanoic acid, 3-methyl-, methy...	130	C7H14O2	002177-78-8	35
2	5-Hexenoic acid, methyl ester	128	C7H12O2	002396-80-7	32
3	Octanoic acid, methyl ester	158	C9H18O2	000111-11-5	27
4	Octanoic acid, 2-methyl-	158	C9H18O2	003004-93-1	27
5	2-Amino-4-methyl-4-pentenoic acid	129	C6H11NO2	1010133-00-5	27





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Misc :
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Instrument : BNA_F
ClientSampleId : DAY-1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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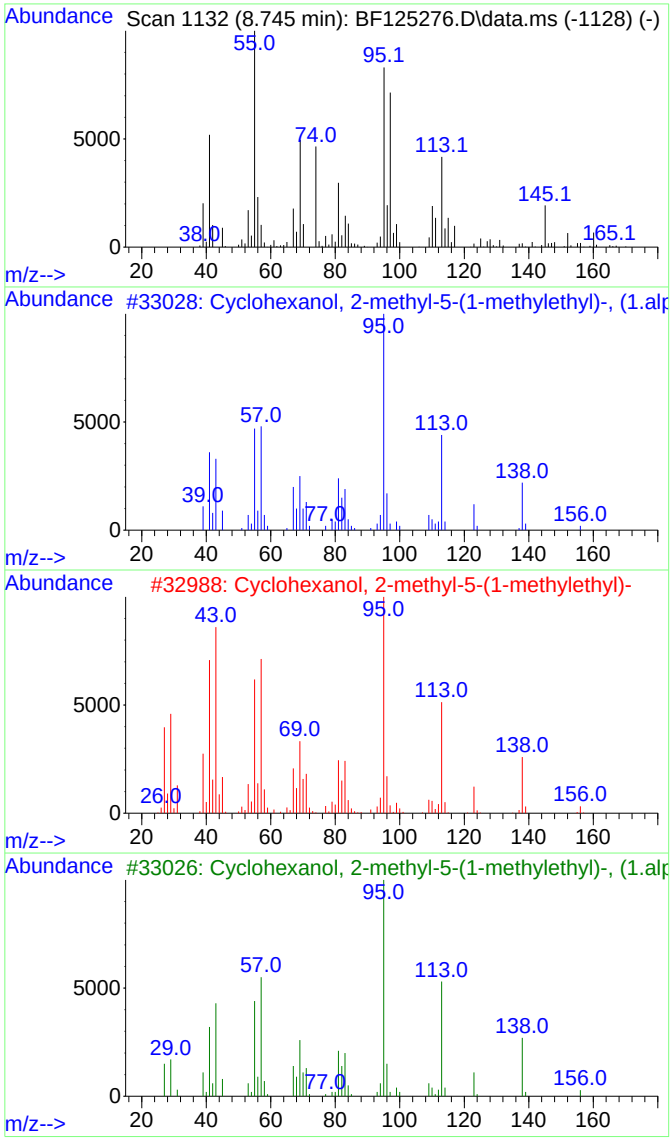
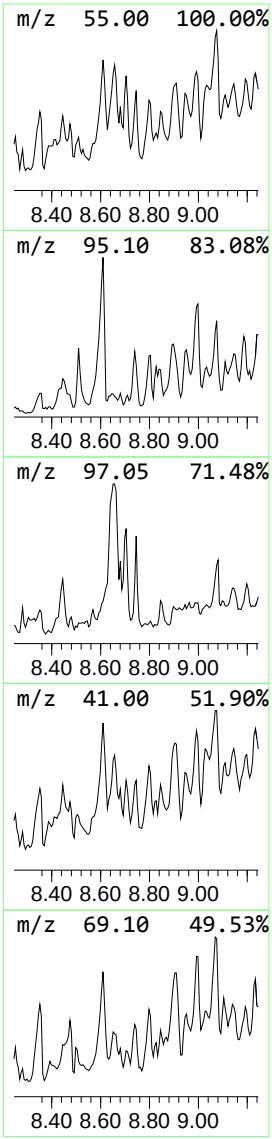
Peak Number 10 unknown8.745 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.745	12.44 ng	956614	Naphthalene-d8	8.198

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanol, 2-methyl-5-(1-meth...	156	C10H20O	000499-69-4	38
2	Cyclohexanol, 2-methyl-5-(1-meth...	156	C10H20O	060320-28-7	38
3	Cyclohexanol, 2-methyl-5-(1-meth...	156	C10H20O	001126-40-5	35
4	Cyclopentane, 1,2-dimethyl-3-met...	110	C8H14	091884-67-2	25
5	Cyclopentene, 1,2,3-trimethyl-	110	C8H14	000473-91-6	22





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Misc :
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Instrument : BNA_F
ClientSampleId : DAY-1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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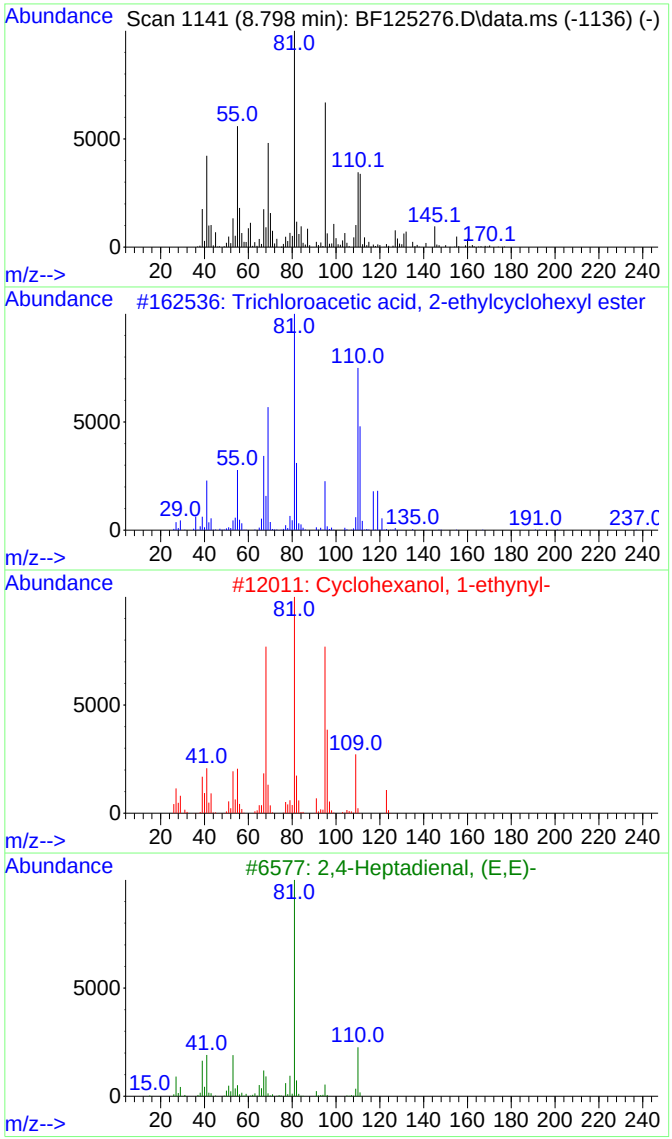
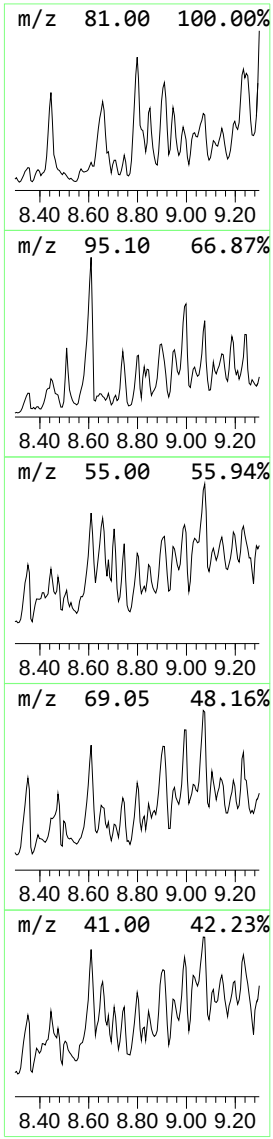
Peak Number 11 unknown8.798 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.798	25.06 ng	1926890	Naphthalene-d8	8.198

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, 2-ethylcyc...	272	C10H15Cl3O2	1000282-57-3	47
2	Cyclohexanol, 1-ethynyl-	124	C8H12O	000078-27-3	43
3	2,4-Heptadienal, (E,E)-	110	C7H10O	004313-03-5	43
4	N-(2-Furylmethyl)-1-butanamine	153	C9H15NO	088230-53-9	35
5	Furan, 2-[(methyldithio)methyl]-	160	C6H8OS2	057500-00-2	27





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Sample : M3561-17
Misc :
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Instrument : BNA_F
ClientSampleId : DAY-1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

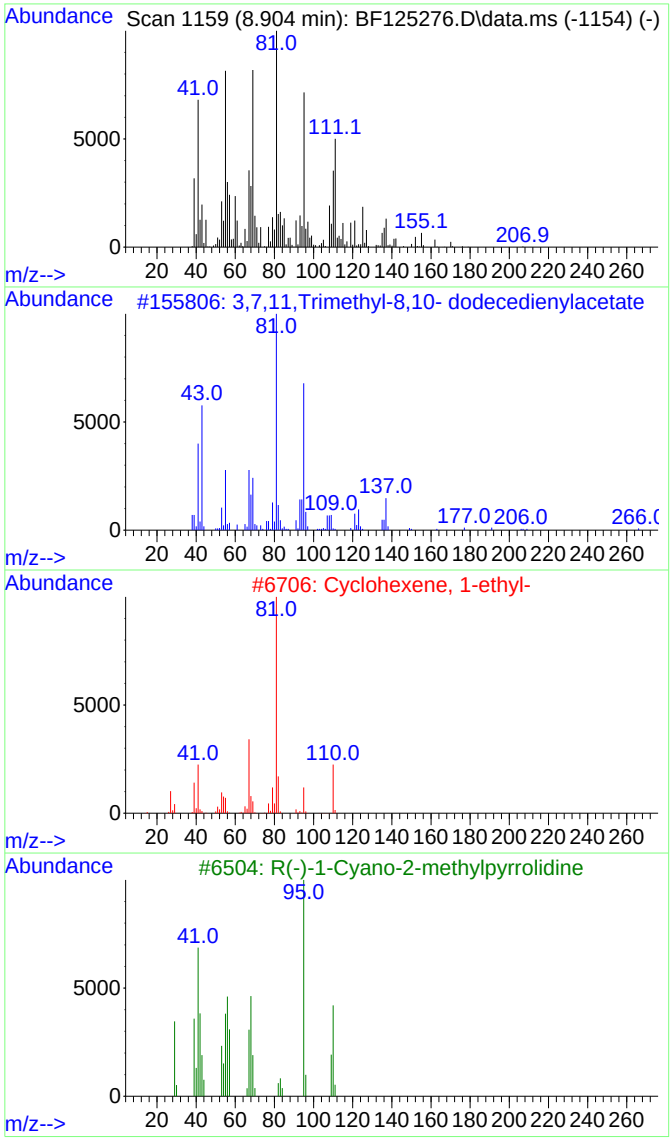
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

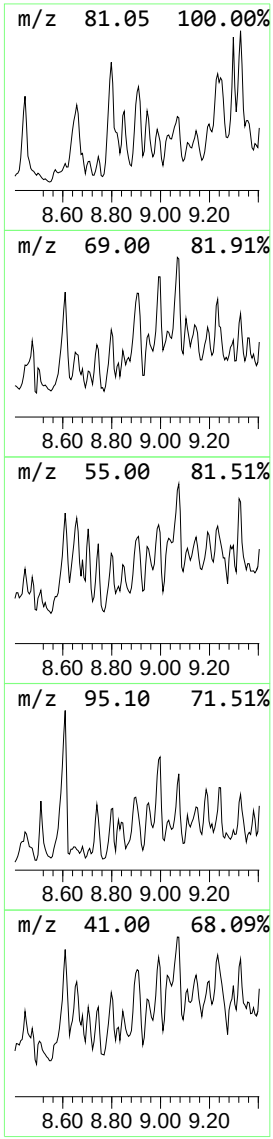
****

Peak Number 12 unknown8.904 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.904	26.84 ng	2063970	Naphthalene-d8	8.198

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,7,11,Trimethyl-8,10- dodecedie...	266	C17H30O2	1000374-10-3	30
2	Cyclohexene, 1-ethyl-	110	C8H14	001453-24-3	25
3	R(-)-1-Cyano-2-methylpyrrolidine	110	C6H10N2	1000145-01-8	25
4	2-Propenyl-3-vinyloxirane	110	C7H10O	070597-49-8	25
5	Benzo[c]thiophene, octahydro-, cis-	142	C8H14S	054053-76-8	25





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Sample : M3561-17
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DAY-1

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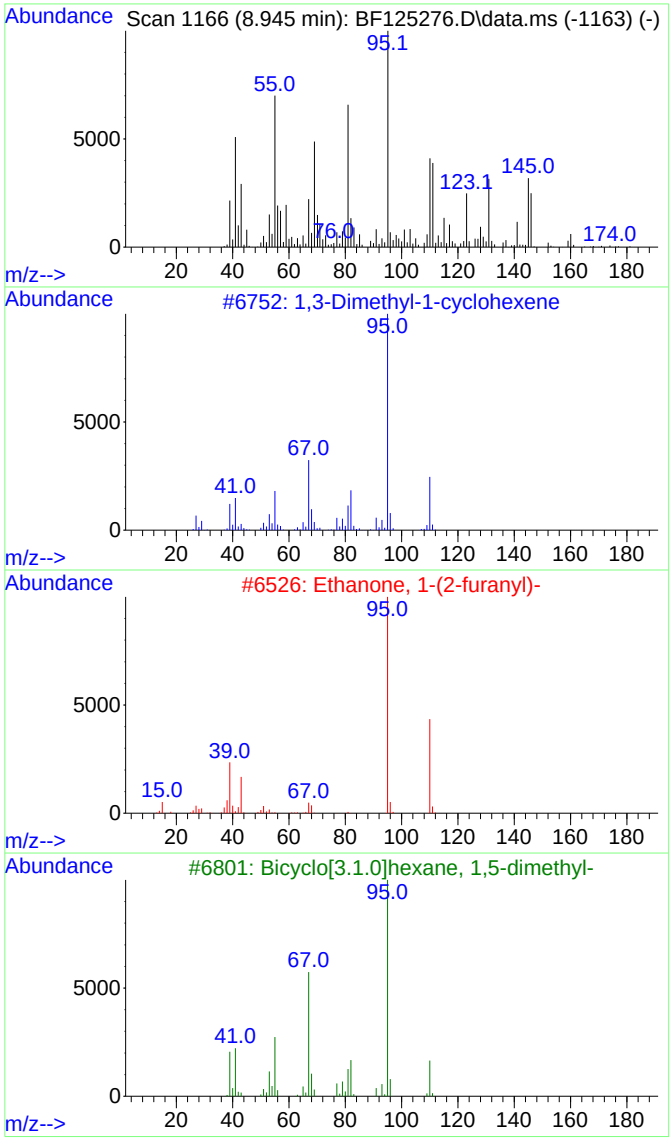
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

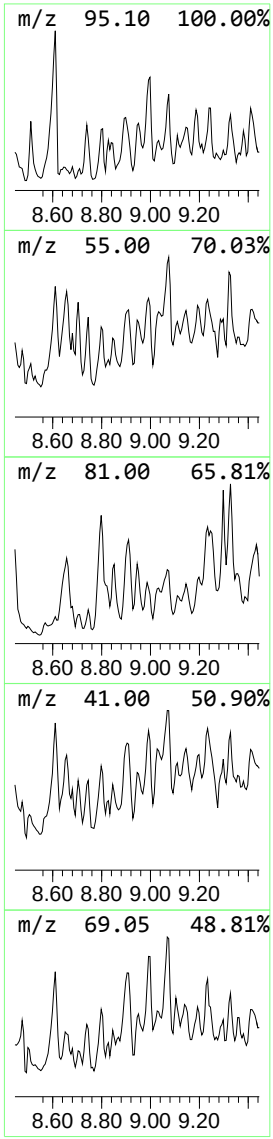
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 unknown8.945 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.945	13.98 ng	1075030	Naphthalene-d8	8.198

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	42
2	Ethanone, 1-(2-furanyl)-	110	C6H6O2	001192-62-7	30
3	Bicyclo[3.1.0]hexane, 1,5-dimethyl-	110	C8H14	1010142-17-5	27
4	trans-3,5-Dimethylcyclohexene	110	C8H14	056021-63-7	27
5	5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	27





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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DAY-1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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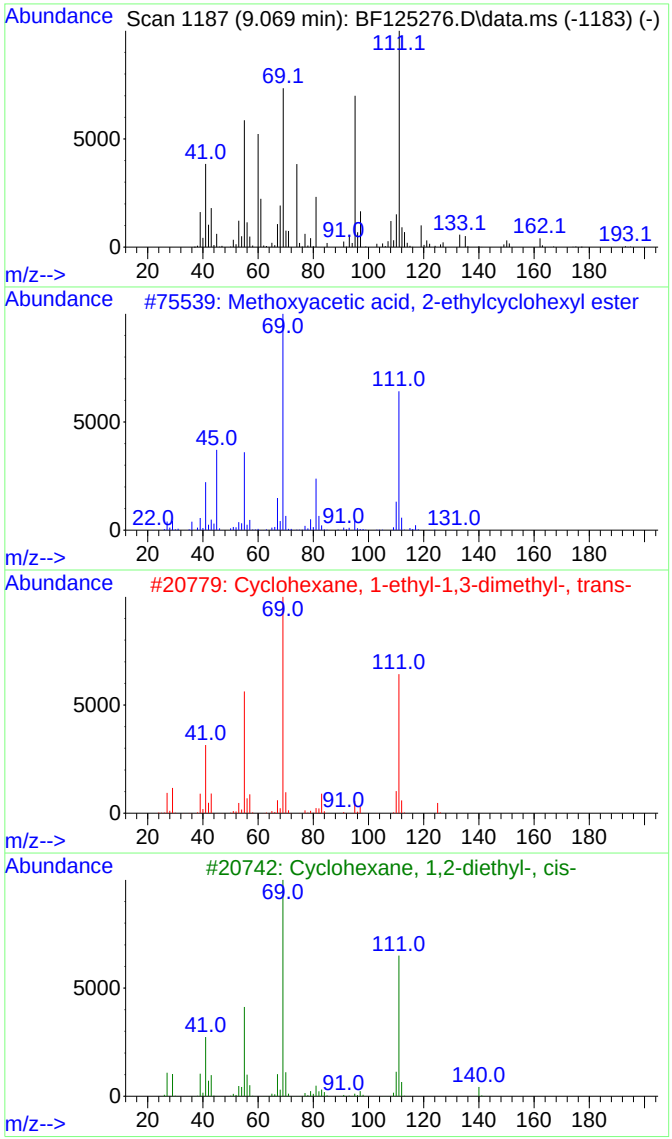
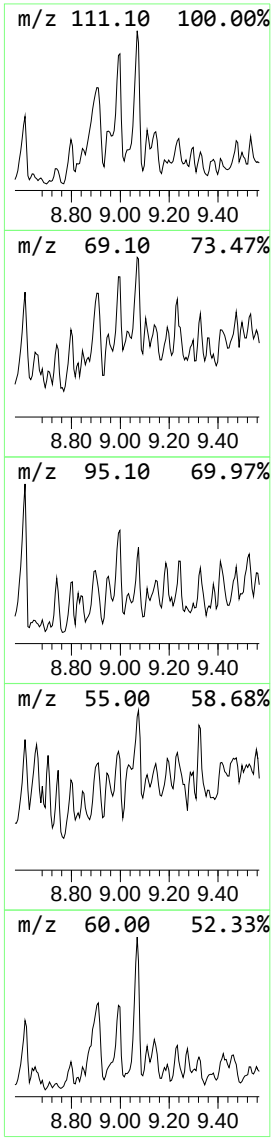
Peak Number 14 unknown9.069 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.069	21.75 ng	1672800	Naphthalene-d8	8.198

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methoxyacetic acid, 2-ethylcyclo...	200	C11H20O3	1000282-69-7	43
2	Cyclohexane, 1-ethyl-1,3-dimethy...	140	C10H20	062238-29-3	43
3	Cyclohexane, 1,2-diethyl-, cis-	140	C10H20	000824-43-1	38
4	Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-27-3	38
5	Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	38





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Instrument : BNA_F
ClientSampleId : DAY-1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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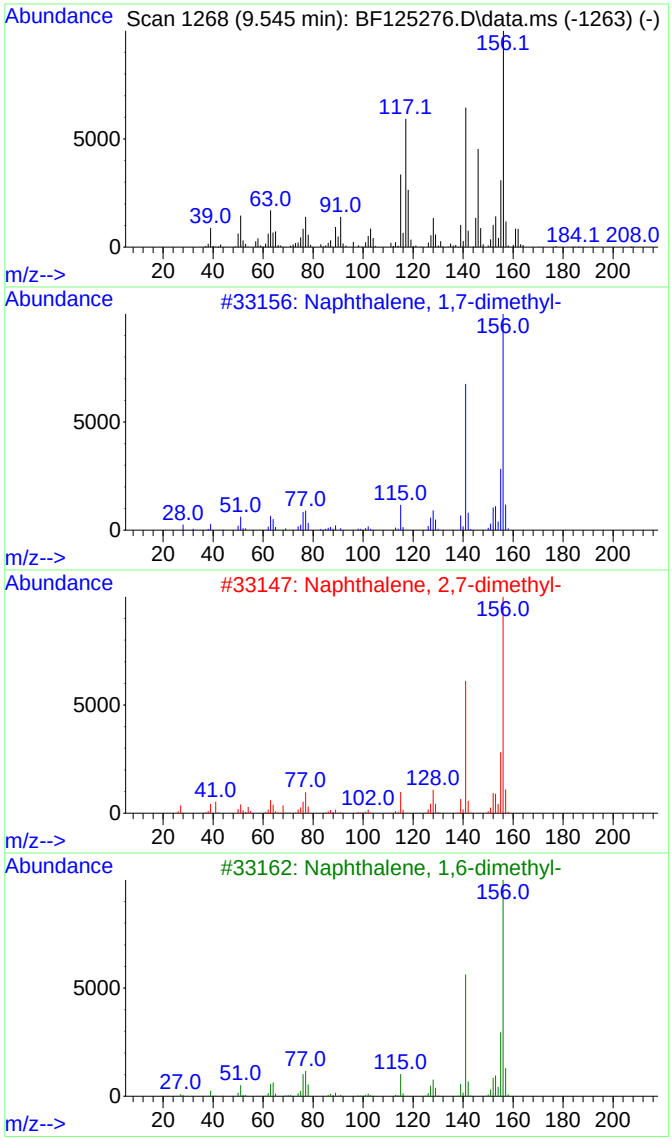
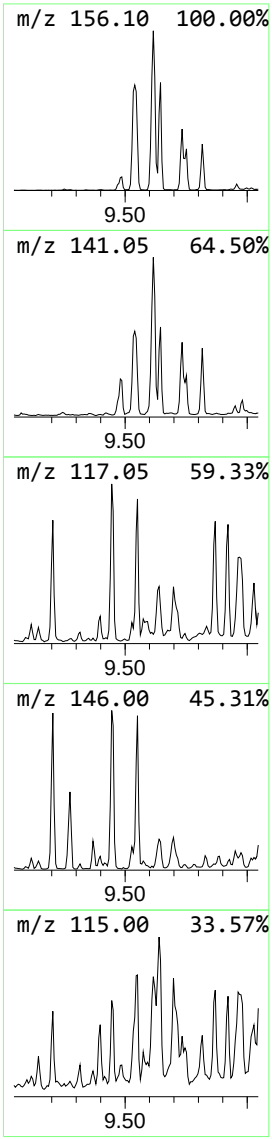
Peak Number 15 Naphthalene, 1,7-dimethyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.545	13.60 ng	3854580	Acenaphthene-d10	9.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	95
2	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	95
3	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	95
4	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	95
5	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	89





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ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DAY-1

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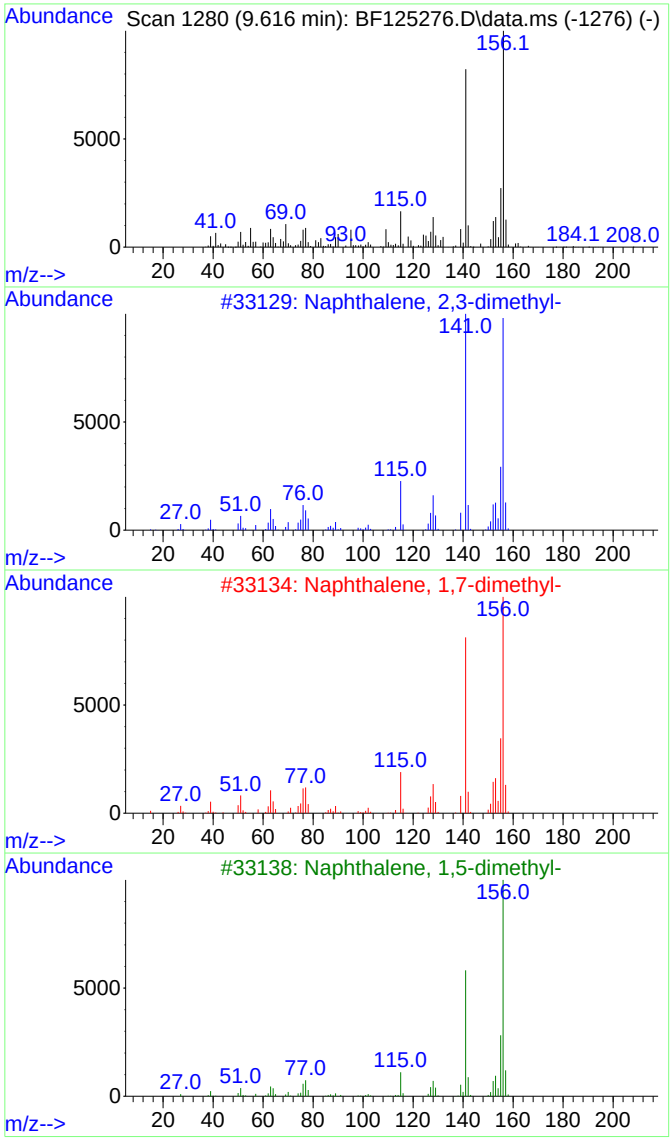
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

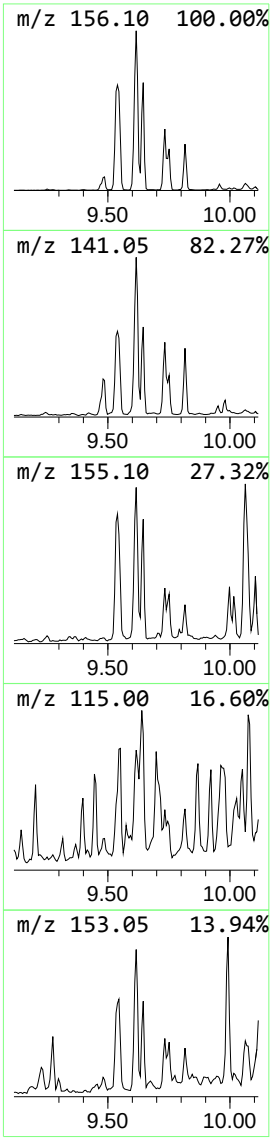
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 16 Naphthalene, 2,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.616	18.22 ng	5164120	Acenaphthene-d10	9.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
2	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	98
3	Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	97
4	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
5	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97





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Data File : BF125276.D
Acq On : 30 Aug 2021 22:37
Operator : JU/CG
Sample : M3561-17
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DAY-1

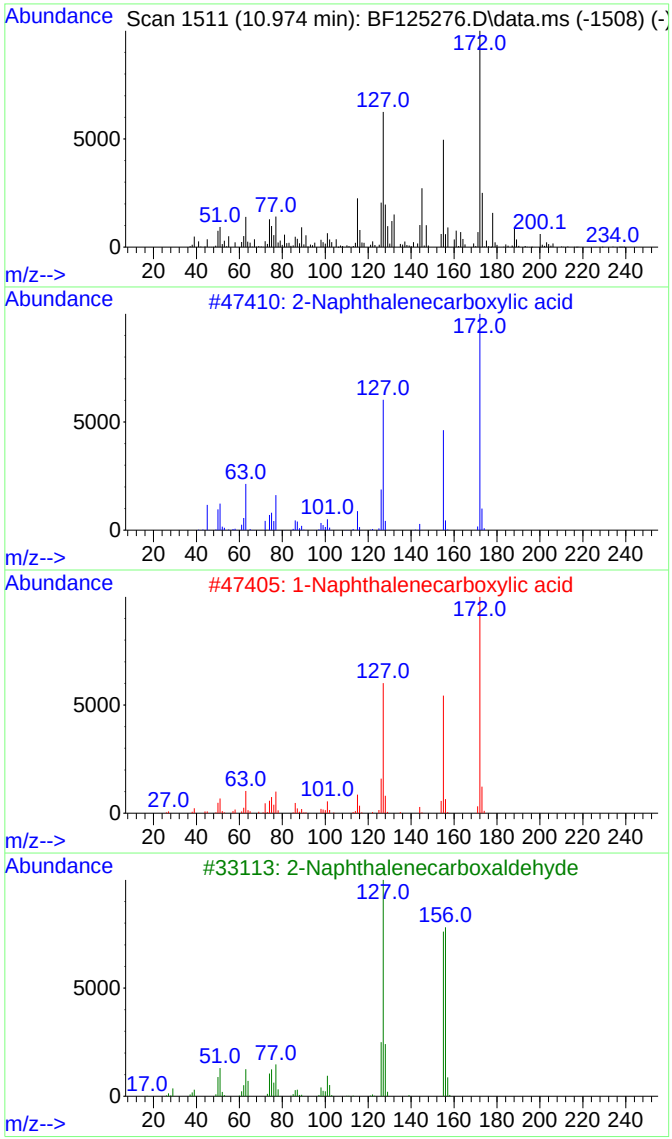
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

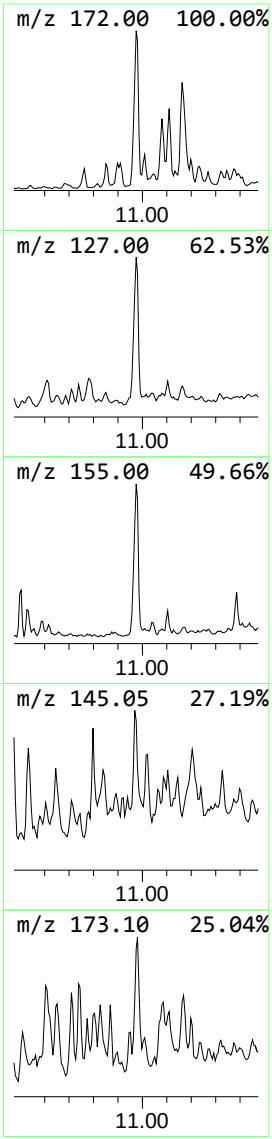
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 17 2-Naphthalenecarboxylic acid Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.975	12.92 ng	2058890	Phenanthrene-d10	11.451

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Naphthalenecarboxylic acid	172	C11H8O2	000093-09-4	92
2	1-Naphthalenecarboxylic acid	172	C11H8O2	000086-55-5	70
3	2-Naphthalenecarboxaldehyde	156	C11H8O	000066-99-9	43
4	6-Phenyl-3(2H)-pyridazinone	172	C10H8N2O	002166-31-6	35
5	Benzene, 1-fluoro-4-(2,2-dicyano...	172	C10H5FN2	002826-22-4	27





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Acq On : 30 Aug 2021 22:37
Operator : JU/CG
Sample : M3561-17
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DAY-1

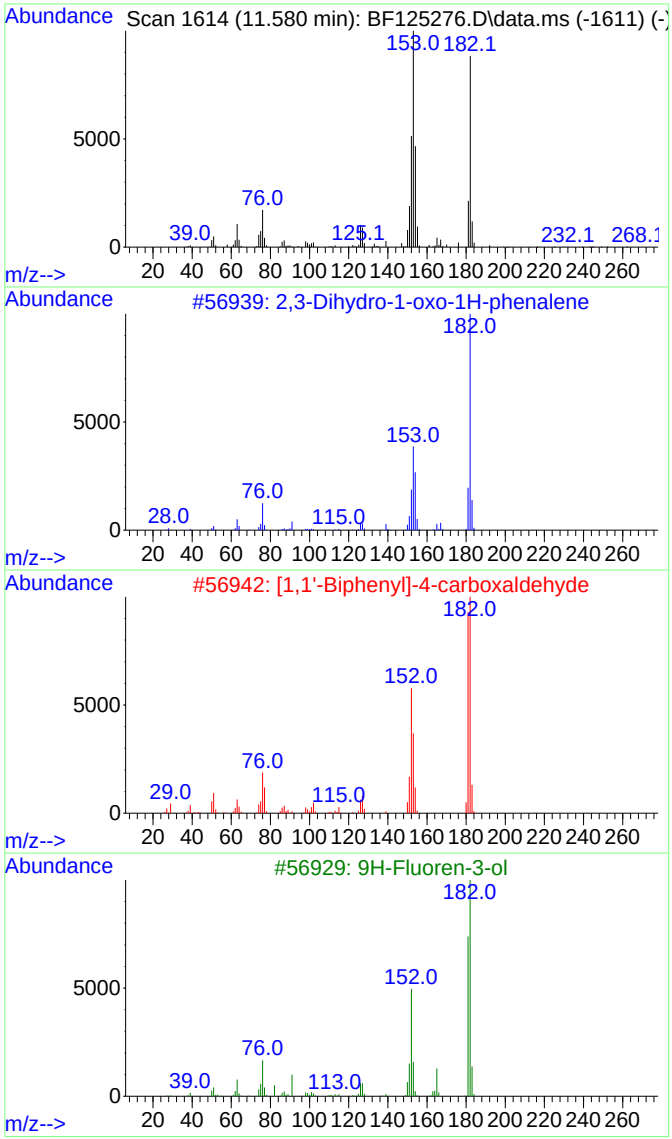
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

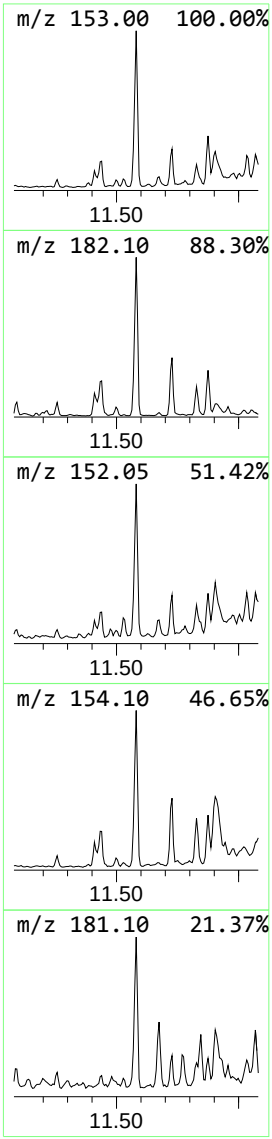
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 18 2,3-Dihydro-1-oxo-1H-phenalene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.580	18.15 ng	2893490	Phenanthrene-d10	11.451

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Dihydro-1-oxo-1H-phenalene	182	C13H10O	000518-85-4	72
2	[1,1'-Biphenyl]-4-carboxaldehyde	182	C13H10O	003218-36-8	49
3	9H-Fluoren-3-ol	182	C13H10O	006344-67-8	43
4	9H-Pyrido[3,4-b]indole, 1-methyl-	182	C12H10N2	000486-84-0	35
5	2(1H)-Pyridinethione, 1-ethyl-4-...	153	C8H11NS	019006-72-5	35





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Data File : BF125276.D
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Operator : JU/CG
Sample : M3561-17
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DAY-1

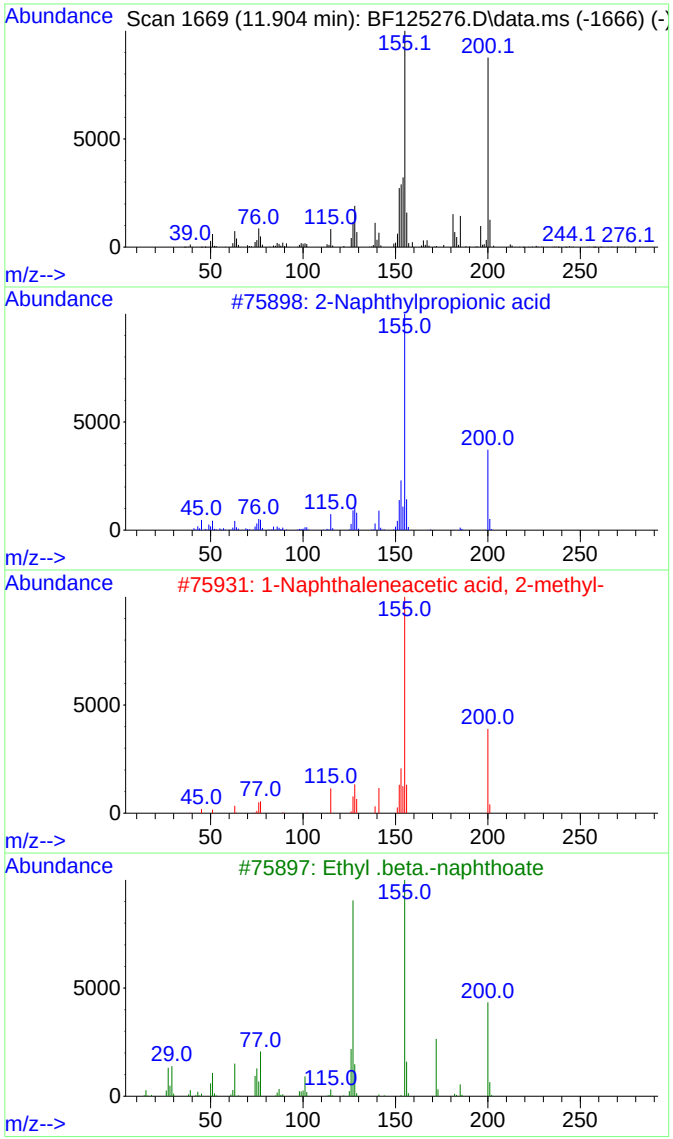
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

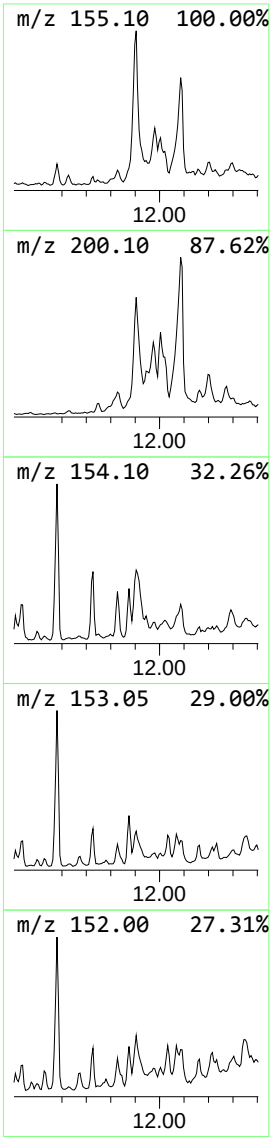
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 19 2-Naphthylpropionic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.904	14.33 ng	2285090	Phenanthrene-d10	11.451

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Naphthylpropionic acid	200	C13H12O2	1000129-24-1	76
2	1-Naphthaleneacetic acid, 2-methyl-	200	C13H12O2	000085-08-5	72
3	Ethyl .beta.-naphthoate	200	C13H12O2	003007-91-8	53
4	1-Naphthaleneacetic acid, .alpha...	200	C12H8O3	026153-26-4	50
5	1-Naphthalenecarboxylic acid, et...	200	C13H12O2	003007-97-4	50





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Acq On : 30 Aug 2021 22:37
Operator : JU/CG
Sample : M3561-17
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DAY-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

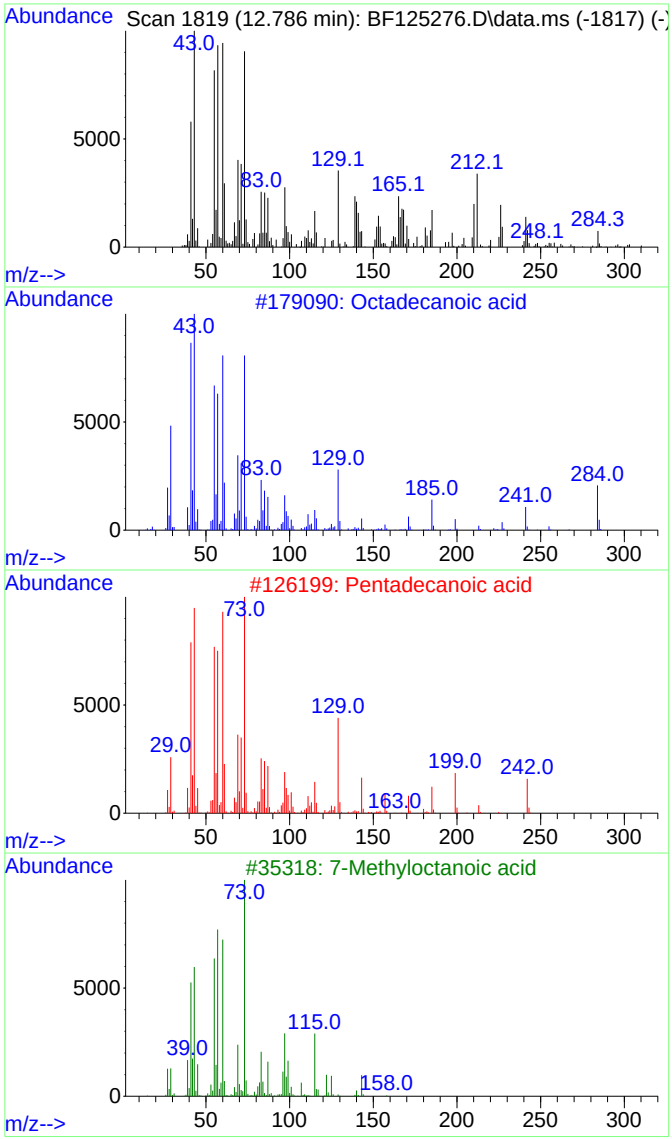
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

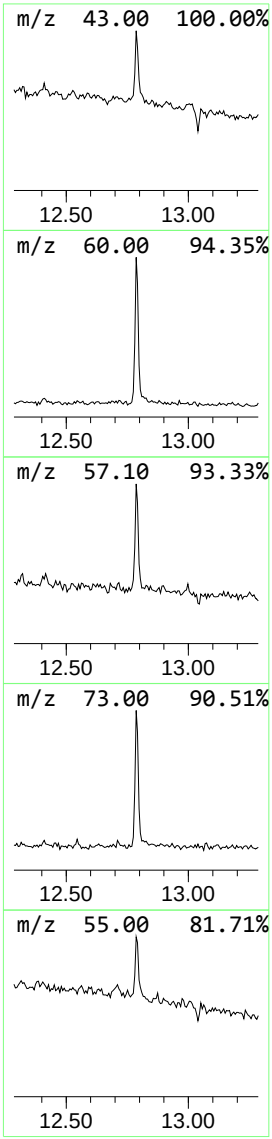
****

Peak Number 20 Octadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.786	14.31 ng	847806	Chrysene-d12	14.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	83
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	27
3	7-Methyloctanoic acid	158	C9H18O2	000693-19-6	27
4	n-Decanoic acid	172	C10H20O2	000334-48-5	27
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083021\
Data File : BF125276.D
Acq On : 30 Aug 2021 22:37
Operator : JU/CG
Sample : M3561-17
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DAY-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.163	36.8	ng	2676830	1	6.916	1453090	20.0
unknown7.351	7.351	13.1	ng	949384	1	6.916	1453090	20.0
unknown7.863	7.863	21.3	ng	1641060	2	8.198	1538080	20.0
unknown8.351	8.351	21.8	ng	1677050	2	8.198	1538080	20.0
9-Methylbicyclo...	8.445	12.7	ng	974140	2	8.198	1538080	20.0
1H-Indene, 2,3-...	8.581	13.1	ng	1003760	2	8.198	1538080	20.0
unknown8.610	8.610	18.9	ng	1453400	2	8.198	1538080	20.0
Benzene, 1-meth...	8.663	25.9	ng	1989230	2	8.198	1538080	20.0
unknown8.704	8.704	10.5	ng	809886	2	8.198	1538080	20.0
unknown8.745	8.745	12.4	ng	956614	2	8.198	1538080	20.0
unknown8.798	8.798	25.1	ng	1926890	2	8.198	1538080	20.0
unknown8.904	8.904	26.8	ng	2063970	2	8.198	1538080	20.0
unknown8.945	8.945	14.0	ng	1075030	2	8.198	1538080	20.0
unknown9.069	9.069	21.8	ng	1672800	2	8.198	1538080	20.0
Naphthalene, 1,...	9.545	13.6	ng	3854580	3	9.957	5668740	20.0
Naphthalene, 2,...	9.616	18.2	ng	5164120	3	9.957	5668740	20.0
2-Naphthaleneca...	10.975	12.9	ng	2058890	4	11.451	3188340	20.0
2,3-Dihydro-1-o...	11.580	18.1	ng	2893490	4	11.451	3188340	20.0
2-Naphthylpropi...	11.904	14.3	ng	2285090	4	11.451	3188340	20.0
Octadecanoic acid	12.786	14.3	ng	847806	5	14.104	1185060	20.0