LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061221\
Data File : BF124287.D
Acq On : 12 Jun 2021 15:37
Operator : JU/CG
Sample : M2674-01 5X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TMR-DS-01-060921

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: BF124287.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	6.492	745	749	753	rVV2	144358	261828	11.24%	0.519%
2	6.663	776	778	782	rVV3	269947	307624	13.20%	0.610%
3	6.839	804	808	811	rBV	316120	272265	11.68%	0.539%
4	6.898	815	818	822	rVV3	186232	214413	9.20%	0.425%
5	6.992	831	834	837	rBV	231663	257512	11.05%	0.510%
6	7.104	848	853	859	rBV3	534541	584238	25.07%	1.158%
7	7.269	876	881	885	rVB	606749	667510	28.64%	1.323%
8	7.381	897	900	902	rVV2	513450	451635	19.38%	0.895%
9	7.404	902	904	907	rVV4	215648	194340	8.34%	0.385%
10	7.487	913	918	921	rVB2	156078	229427	9.85%	0.455%
11	7.534	921	926	930	rBV4	350866	506747	21.75%	1.004%
12	7.575	930	933	942	rVB	478704	562438	24.14%	1.114%
13	7.698	949	954	957	rBV2	154450	222969	9.57%	0.442%
14	7.804	966	972	976	rVB2	605554	971875	41.71%	1.926%
15	7.863	979	982	986	rBV3	196858	244175	10.48%	0.484%
16	7.928	991	993	998	rVB2	611752	611408	26.24%	1.211%
17	7.992	998	1004	1011	rVB3	346267	534060	22.92%	1.058%
18	8.057	1011	1015	1018	rBV3	290157	350157	15.03%	0.694%
19	8.092	1018	1021	1025	rBV2	858599	916415	39.33%	1.816%
20	8.128	1025	1027	1029	rVV	255004	178933	7.68%	0.355%
21	8.145	1029	1030	1033	rVB	396018	288134	12.36%	0.571%
22	8.198	1035	1039	1042	rBV3	255824	259905	11.15%	0.515%
23	8.228	1042	1044	1047	rBV2	219637	218817	9.39%	0.434%
24	8.298	1051	1056	1059	rBV2	648947	891796	38.27%	1.767%
25	8.369	1065	1068	1071	rVB	299571	276651	11.87%	0.548%
26	8.492	1085	1089	1091	rBV	744154	655391	28.12%	1.299%
27	8.569	1098	1102	1104	rBV2	218376	284945	12.23%	0.565%
28	8.592	1104	1106	1108	rVV	352613	247693	10.63%	0.491%
29	8.628	1108	1112	1114	rVV	802023	882051	37.85%	1.748%
30	8.781	1135	1138	1140	rBV2	205421	217252	9.32%	0.430%
31	8.845	1146	1149	1150	rBV	671010	560486	24.05%	1.111%
32	8.863	1150	1152	1153	rVV2	267773	258363	11.09%	0.512%
33	8.904	1156	1159	1163	rVB3	373658	517078	22.19%	1.025%
34	8.939	1163	1165	1168	rBV2	481807	369426	15.85%	0.732%
35	9.022	1176	1179	1180	rBV3	274469	298444	12.81%	0.591%
36	9.045	1180	1183	1186	rVB	1280929	1292087	55.45%	2.560%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061221\
Data File : BF124287.D
Acq On : 12 Jun 2021 15:37
Operator : JU/CG
Sample : M2674-01 5X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TMR-DS-01-060921

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	9.139	1195	1199	1202	rVB	742213	749354	32.16%	1.485%
38	9.198	1206	1209	1212	rVB2	255359	285224	12.24%	0.565%
39	9.239	1212	1216	1217	rBV2	197223	256863	11.02%	0.509%
40	9.281	1220	1223	1225	rBV3	395203	291846	12.52%	0.578%
41	9.375	1235	1239	1241	rVB3	144840	182004	7.81%	0.361%
42	9.398	1241	1243	1247	rBV4	160831	177245	7.61%	0.351%
43	9.475	1251	1256	1259	rBV4	428520	768452	32.98%	1.523%
44	9.563	1265	1271	1275	rVB2	1772396	2330307	100.00%	4.617%
45	9.616	1275	1280	1282	rBV3	400646	477137	20.48%	0.945%
46	9.810	1309	1313	1315	rBV3	417455	530517	22.77%	1.051%
47	9.886	1323	1326	1328	rBV	358452	267827	11.49%	0.531%
48	9.963	1333	1339	1342	rBV	1783133	1984289	85.15%	3.932%
49	10.028	1347	1350	1353	rBV	208964	194758	8.36%	0.386%
50	10.069	1353	1357	1358	rBV3	241248	358177	15.37%	0.710%
51	10.086	1358	1360	1363	rVB2	374765	301677	12.95%	0.598%
52	10.233	1382	1385	1389	rVB6	178128	210592	9.04%	0.417%
53	10.280	1389	1393	1395	rBV4	360212	446031	19.14%	0.884%
54	10.310	1395	1398	1400	rVB2	411939	390374	16.75%	0.774%
55	10.339	1400	1403	1406	rBV3	284044	313183	13.44%	0.621%
56	10.380	1406	1410	1413	rBV	1783811	1506401	64.64%	2.985%
57	10.433	1416	1419	1423	rVB2	257562	294436	12.64%	0.583%
58	10.586	1441	1445	1449	rVV5	244151	383546	16.46%	0.760%
59	10.627	1449	1452	1455	rVV4	212582	289359	12.42%	0.573%
60	10.663	1455	1458	1464	rVB4	519523	751068	32.23%	1.488%
61	10.780	1477	1478	1483	rVB3	283471	301209	12.93%	0.597%
62	10.839	1483	1488	1491	rBV3	750116	727298	31.21%	1.441%
63	10.998	1508	1515	1517	rBV2	1083203	1534717	65.86%	3.041%
64	11.110	1529	1534	1535	rBV4	186898	275328	11.82%	0.546%
65	11.139	1535	1539	1542	rVB	551535	633662	27.19%	1.256%
66	11.233	1552	1555	1556	rBV2	236497	214080	9.19%	0.424%
67	11.292	1562	1565	1570	rVB2	241896	260269	11.17%	0.516%
68	11.398	1576	1583	1586	rBV3	620183	900828	38.66%	1.785%
69	11.486	1595	1598	1603	rBV6	206792	246172	10.56%	0.488%
70	11.663	1625	1628	1630	rBV	256623	232950	10.00%	0.462%
71	11.763	1643	1645	1649	rVB5	171314	186443	8.00%	0.369%
72	11.916	1667	1671	1674	rBV2	667412	709450	30.44%	1.406%
73	12.069	1695	1697	1703	rVB	296091	312648	13.42%	0.620%
74	12.457	1761	1763	1767	rVB	392451	325601	13.97%	0.645%
75	12.616	1788	1790	1792	rBV2	171793	185079	7.94%	0.367%
76	12.816	1821	1824	1825	rBV	701530	694783	29.82%	1.377%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061221\
Data File : BF124287.D
Acq On : 12 Jun 2021 15:37
Operator : JU/CG
Sample : M2674-01 5X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TMR-DS-01-060921

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	12.827	1825	1826	1831	rVB2	570579	479052	20.56%	0.949%
78	13.186	1885	1887	1889	rVB	254017	176808	7.59%	0.350%
79	13.416	1923	1926	1928	rBV2	249760	222873	9.56%	0.442%
80	13.439	1928	1930	1935	rVB	247536	245322	10.53%	0.486%
81	13.516	1940	1943	1950	rVB2	672432	893435	38.34%	1.770%
82	13.863	1998	2002	2008	rVB	1541737	1692693	72.64%	3.354%
83	13.951	2015	2017	2021	rVB	400245	358718	15.39%	0.711%
84	14.027	2027	2030	2032	rBV	299262	257111	11.03%	0.509%
85	14.086	2036	2040	2043	rVV2	880416	1075962	46.17%	2.132%
86	14.121	2043	2046	2050	rVV2	315708	369226	15.84%	0.732%
87	14.168	2051	2054	2057	rVV3	423798	564078	24.21%	1.118%
88	14.204	2058	2060	2063	rVB	295619	227146	9.75%	0.450%
89	14.498	2106	2110	2115	rVB	1280045	1337502	57.40%	2.650%
90	14.568	2119	2122	2126	rVB2	262185	294864	12.65%	0.584%
91	14.710	2141	2146	2149	rBV3	552750	750980	32.23%	1.488%
92	14.833	2162	2167	2170	rVB	239664	393073	16.87%	0.779%
93	15.168	2221	2224	2231	rVB5	134024	203319	8.72%	0.403%
94	15.757	2320	2324	2329	rVB2	288227	378650	16.25%	0.750%
95	15.921	2348	2352	2359	rVV8	200293	322075	13.82%	0.638%
96	15.998	2360	2365	2370	rVV3	543518	836206	35.88%	1.657%
97	16.227	2396	2404	2412	rVB6	457257	1074370	46.10%	2.129%
98	17.568	2626	2632	2640	rBV6	90630	261594	11.23%	0.518%
99	18.374	2765	2769	2779	rVB6	83244	203466	8.73%	0.403%
100	18.603	2803	2808	2818	rVB10	115981	309229	13.27%	0.613%

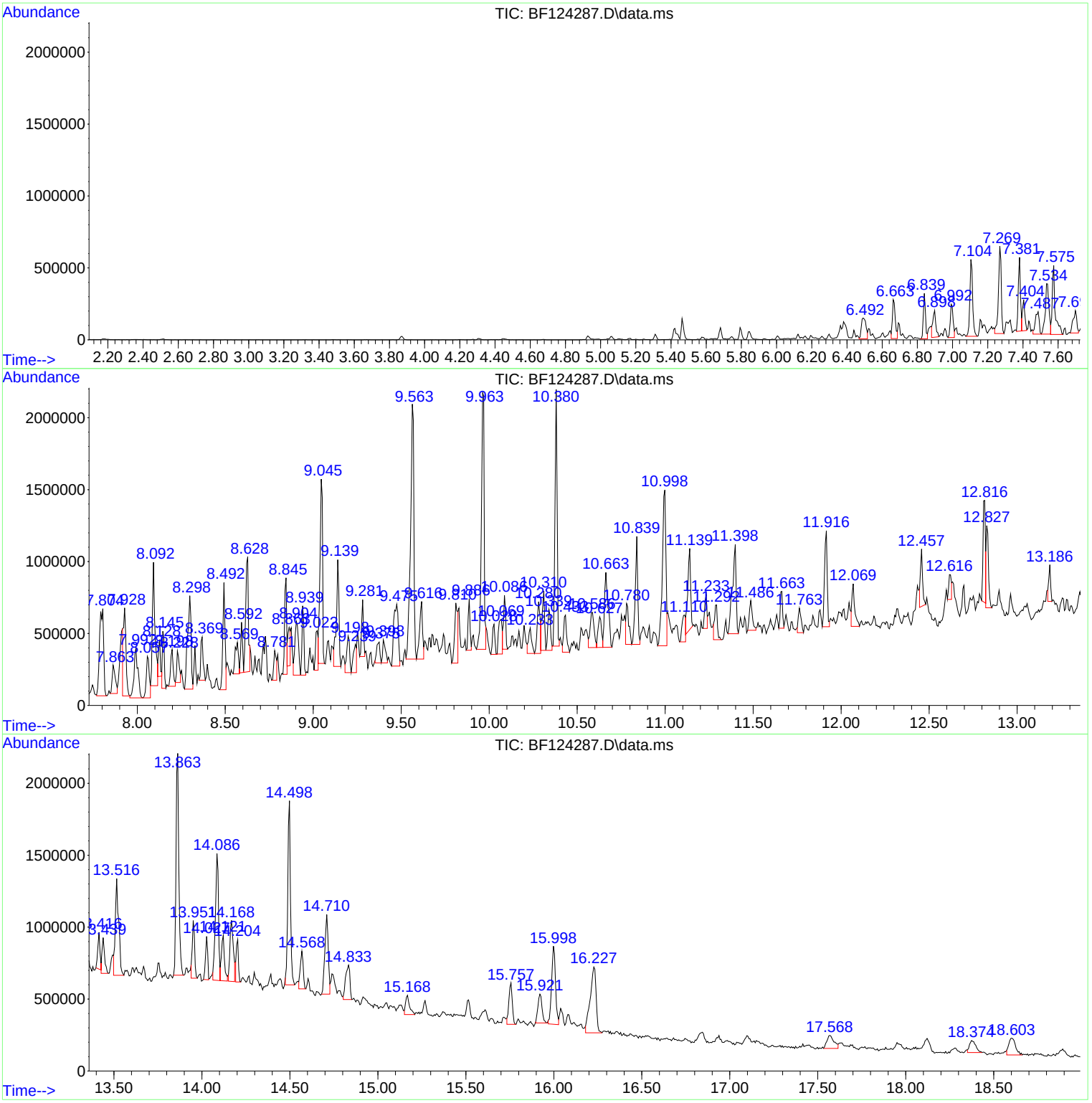
Sum of corrected areas: 50467424

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061221\
Data File : BF124287.D
Acq On : 12 Jun 2021 15:37
Operator : JU/CG
Sample : M2674-01 5X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TMR-DS-01-060921

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 : BF124287.D
Acq On : 12 Jun 2021 15:37
Operator : JU/CG
Sample : M2674-01 5X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TMR-DS-01-060921

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

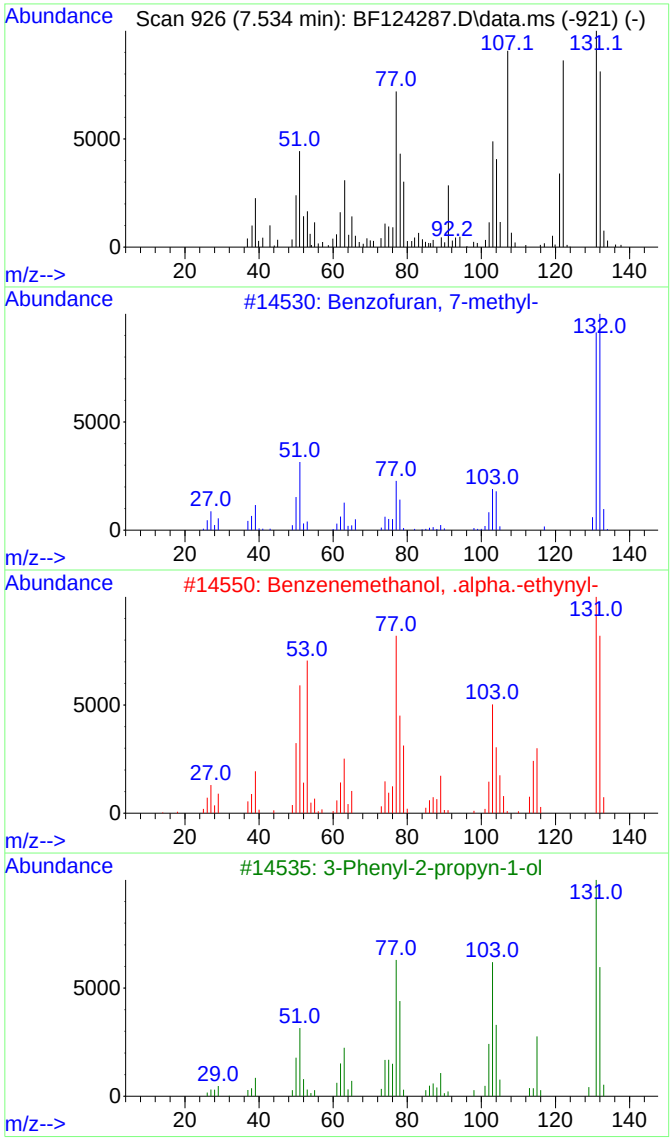
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

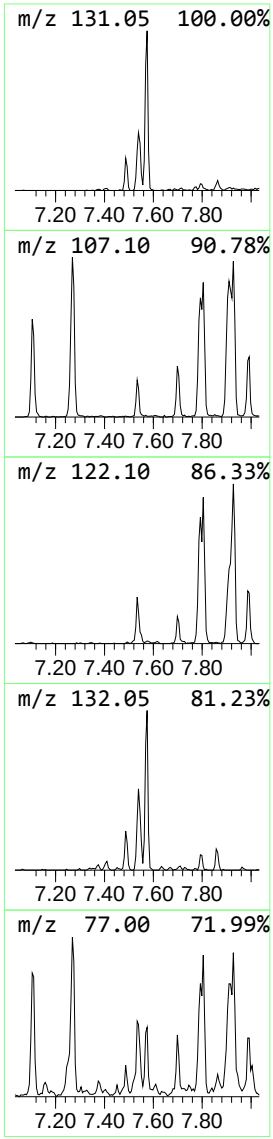
****

Peak Number 1 Benzofuran, 7-methyl- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.534	56.64 ng	506747	Naphthalene-d8	8.128

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzofuran, 7-methyl-	132	C9H8O	017059-52-8	86
2	Benzenemethanol, .alpha.-ethynyl-	132	C9H8O	004187-87-5	83
3	3-Phenyl-2-propyn-1-ol	132	C9H8O	001504-58-1	64
4	Benzofuran, 2-methyl-	132	C9H8O	004265-25-2	64
5	2-Propenal, 3-phenyl-	132	C9H8O	000104-55-2	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061221\
Data File : BF124287.D
Acq On : 12 Jun 2021 15:37
Operator : JU/CG
Sample : M2674-01 5X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TMR-DS-01-060921

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

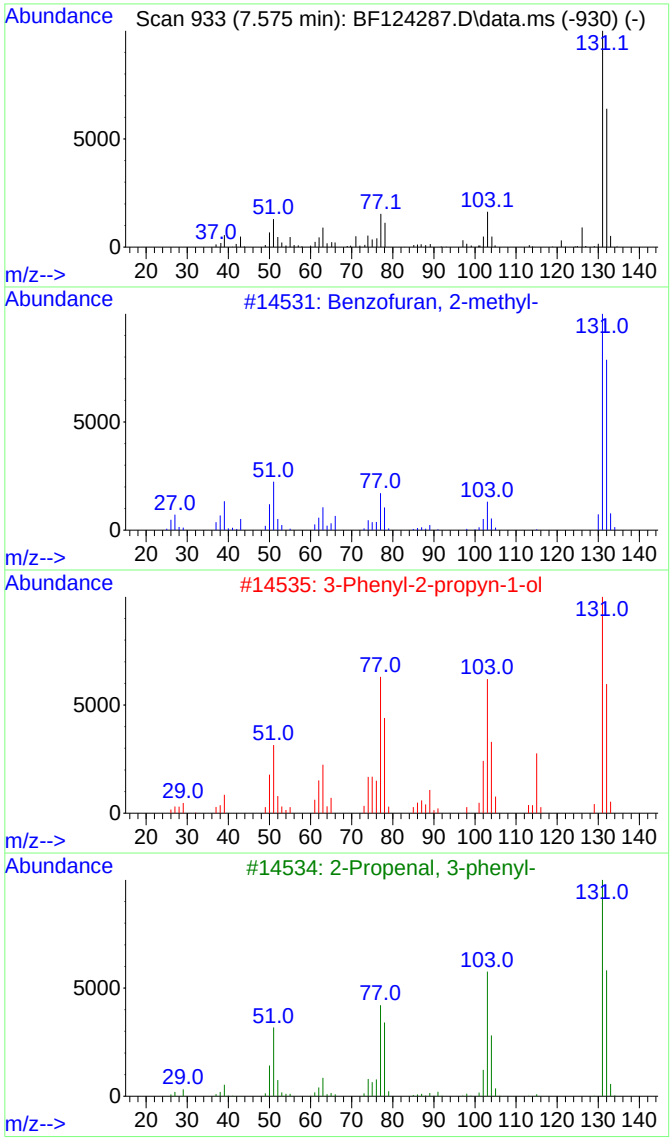
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

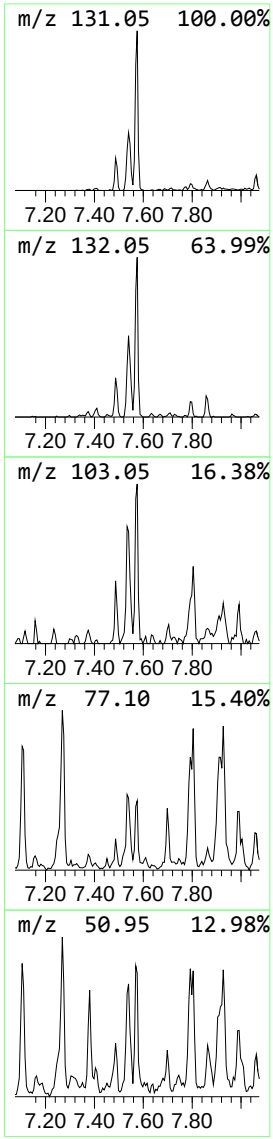
****

Peak Number 2 Benzofuran, 2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.575	62.87 ng	562438	Naphthalene-d8	8.128

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzofuran, 2-methyl-	132	C9H8O	004265-25-2	94
2	3-Phenyl-2-propyn-1-ol	132	C9H8O	001504-58-1	87
3	2-Propenal, 3-phenyl-	132	C9H8O	000104-55-2	86
4	Cinnamaldehyde, (E)-	132	C9H8O	014371-10-9	72
5	Benzopyrimidine, 3,4-dihydro-	132	C8H8N2	001904-64-9	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061221\
Data File : BF124287.D
Acq On : 12 Jun 2021 15:37
Operator : JU/CG
Sample : M2674-01 5X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TMR-DS-01-060921

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

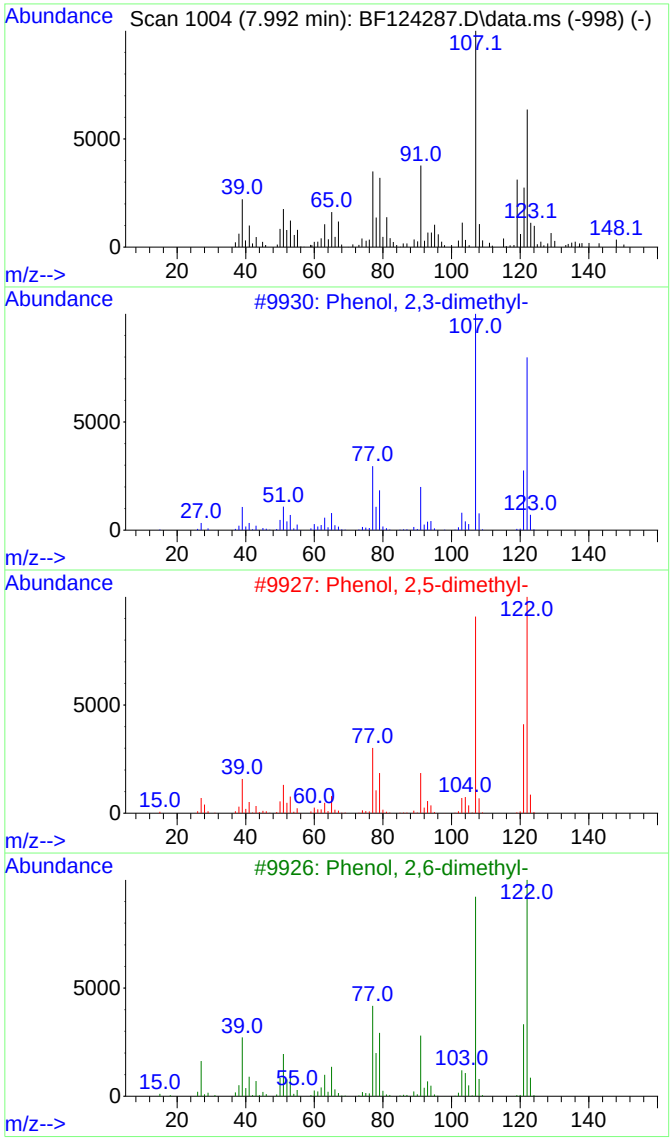
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

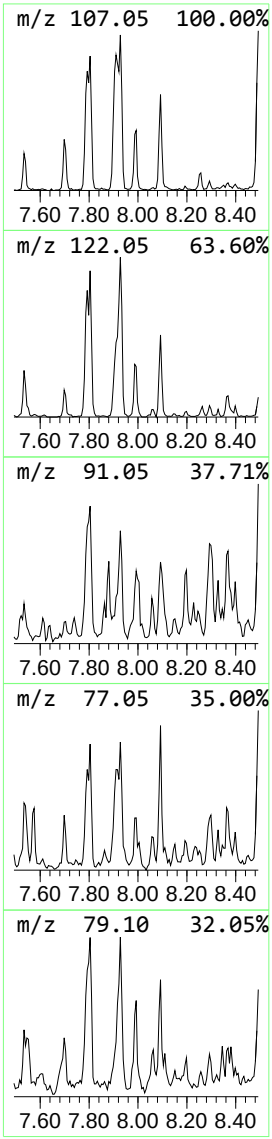
****

Peak Number 3 Phenol, 2,3-dimethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.992	59.69 ng	534060	Naphthalene-d8	8.128

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,3-dimethyl-	122	C8H10O	000526-75-0	93
2	Phenol, 2,5-dimethyl-	122	C8H10O	000095-87-4	81
3	Phenol, 2,6-dimethyl-	122	C8H10O	000576-26-1	78
4	Phenol, 2,4-dimethyl-	122	C8H10O	000105-67-9	70
5	Phenol, 3,5-dimethyl-	122	C8H10O	000108-68-9	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061221\
Data File : BF124287.D
Acq On : 12 Jun 2021 15:37
Operator : JU/CG
Sample : M2674-01 5X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TMR-DS-01-060921

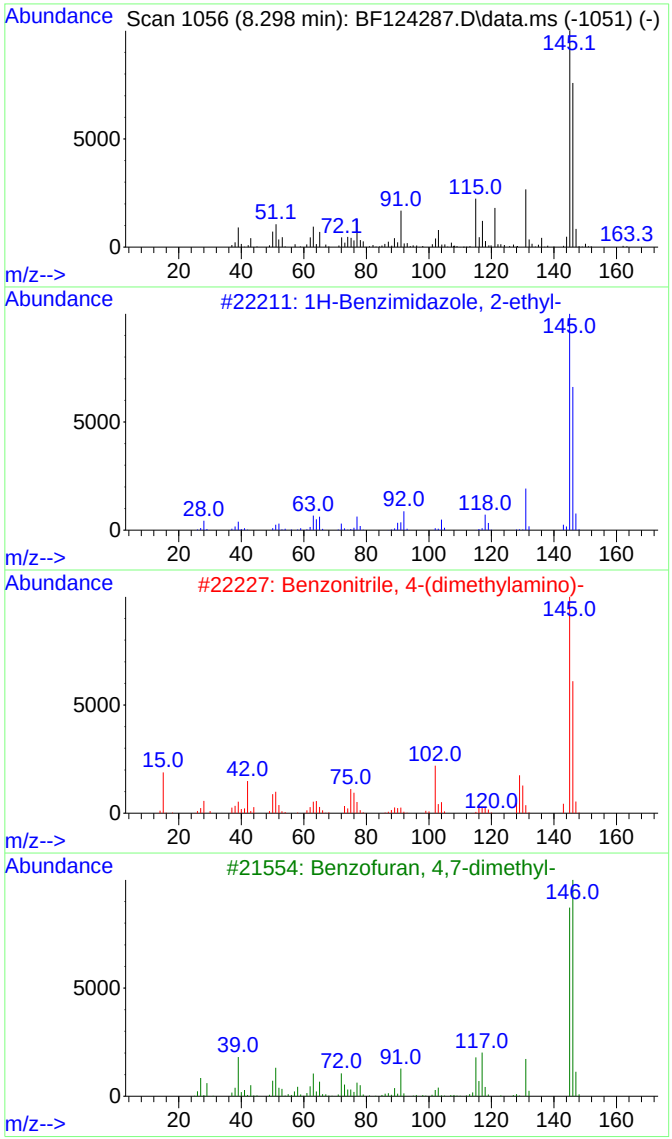
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

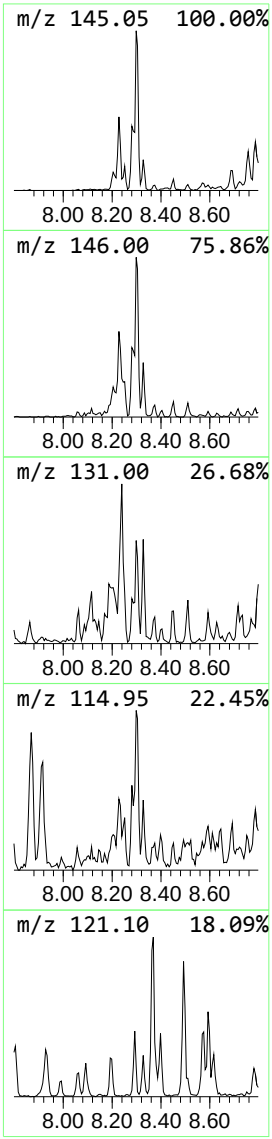
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1H-Benzimidazole, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.298	99.68 ng	891796	Naphthalene-d8	8.128

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzimidazole, 2-ethyl-	146	C9H10N2	001848-84-6	72
2	Benzonitrile, 4-(dimethylamino)-	146	C9H10N2	001197-19-9	53
3	Benzofuran, 4,7-dimethyl-	146	C10H10O	028715-26-6	52
4	1H-Benzimidazole, 5,6-dimethyl-	146	C9H10N2	000582-60-5	47
5	2-Propyn-1-ol, 3-(4-methylphenyl)-	146	C10H10O	016017-24-6	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061221\
Data File : BF124287.D
Acq On : 12 Jun 2021 15:37
Operator : JU/CG
Sample : M2674-01 5X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TMR-DS-01-060921

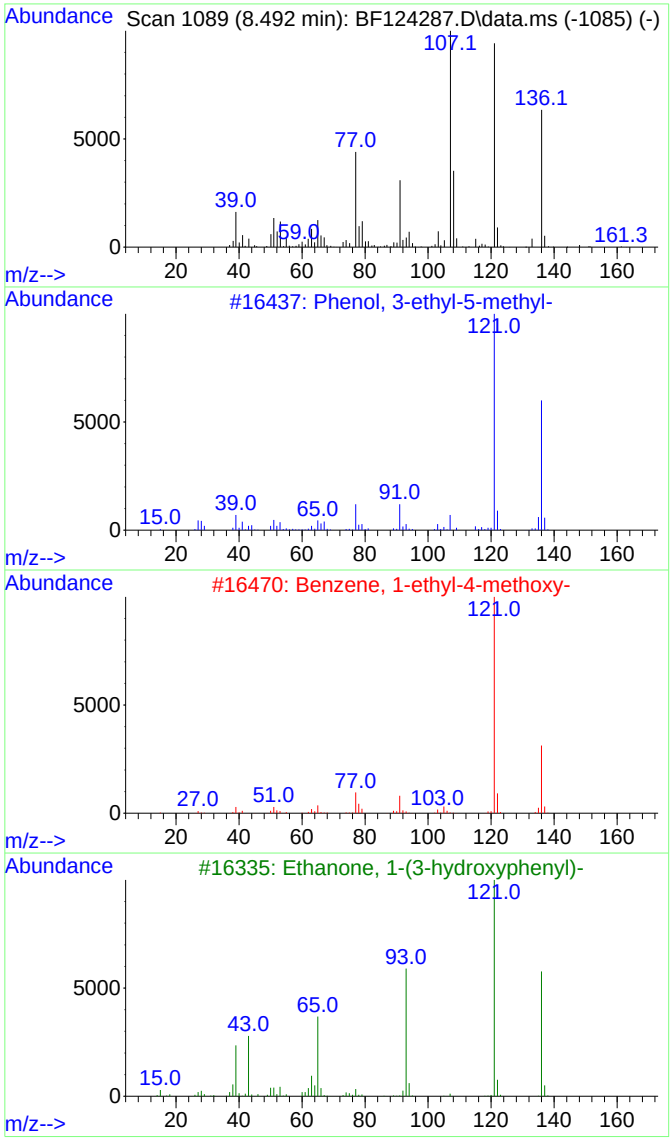
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

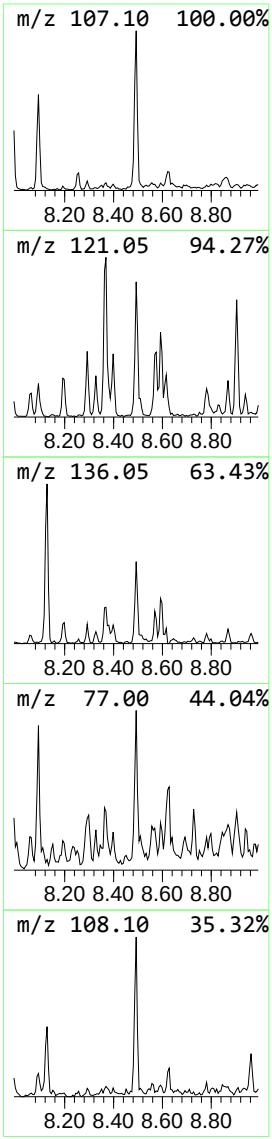
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Phenol, 3-ethyl-5-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.492	73.26 ng	655391	Naphthalene-d8	8.128

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 3-ethyl-5-methyl-	136	C9H12O	000698-71-5	52
2	Benzene, 1-ethyl-4-methoxy-	136	C9H12O	001515-95-3	49
3	Ethanone, 1-(3-hydroxyphenyl)-	136	C8H8O2	000121-71-1	46
4	Phenol, 2,4,5-trimethyl-	136	C9H12O	000496-78-6	45
5	Phenol, 2,3,6-trimethyl-	136	C9H12O	002416-94-6	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061221\
Data File : BF124287.D
Acq On : 12 Jun 2021 15:37
Operator : JU/CG
Sample : M2674-01 5X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TMR-DS-01-060921

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

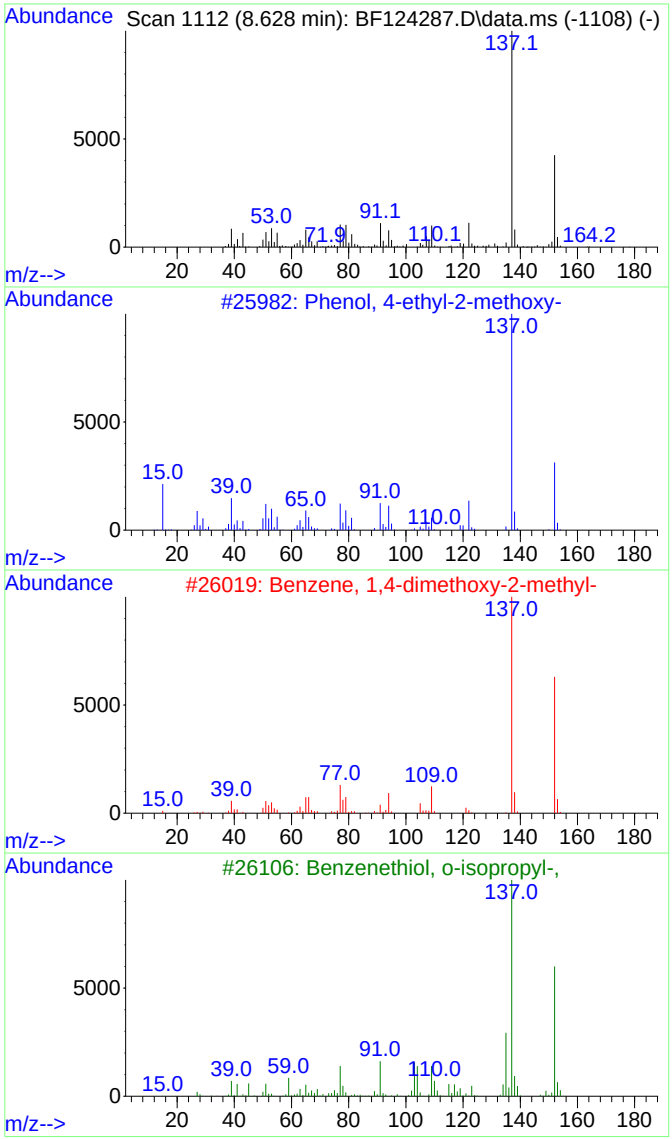
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

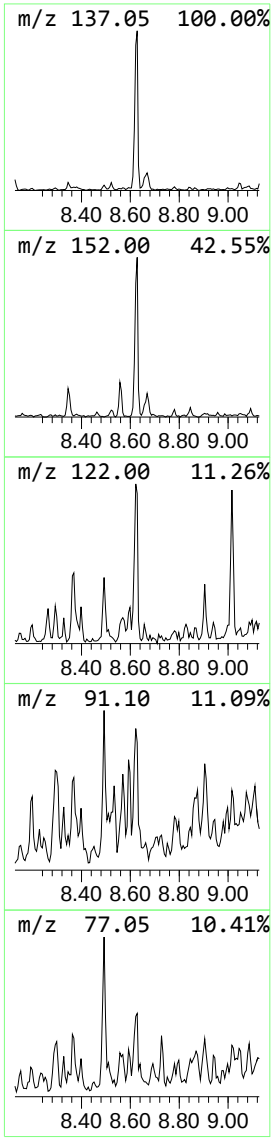
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.628	98.59 ng	882051	Naphthalene-d8	8.128

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-ethyl-2-methoxy-	152	C9H12O2	002785-89-9	91
2	Benzene, 1,4-dimethoxy-2-methyl-	152	C9H12O2	024599-58-4	83
3	Benzenethiol, o-isopropyl-,	152	C9H12S	006262-87-9	72
4	4-Isopropylthiophenol	152	C9H12S	004946-14-9	72
5	2-(2,2-Dimethylcyclopropyl)thiop...	152	C9H12S	005919-16-4	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061221\
Data File : BF124287.D
Acq On : 12 Jun 2021 15:37
Operator : JU/CG
Sample : M2674-01 5X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TMR-DS-01-060921

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

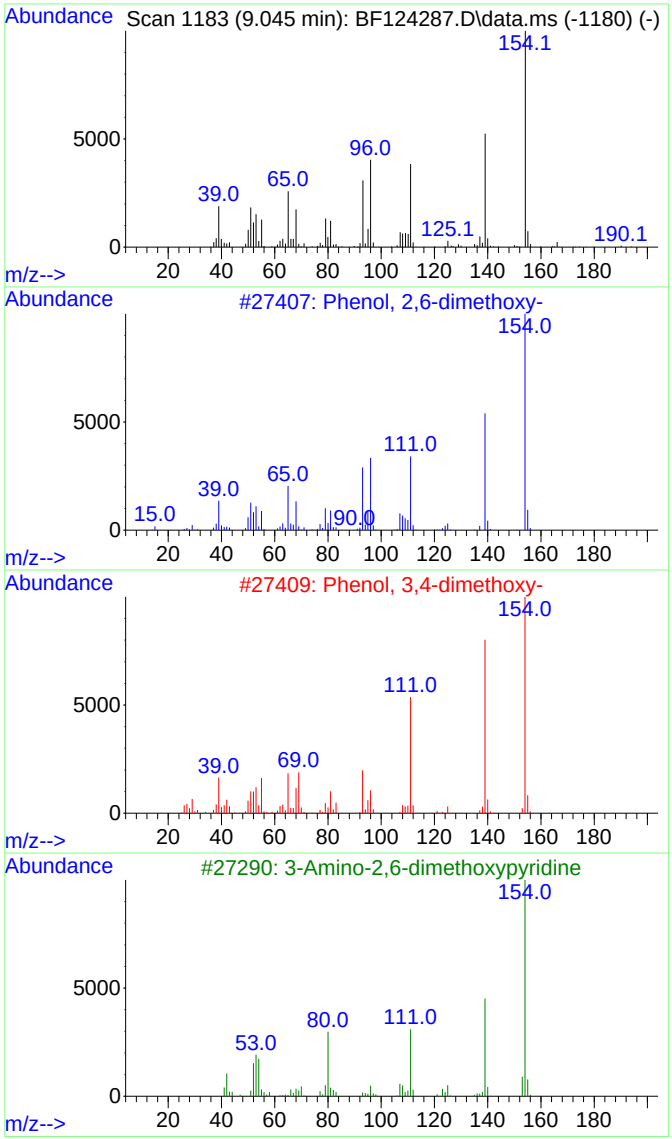
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

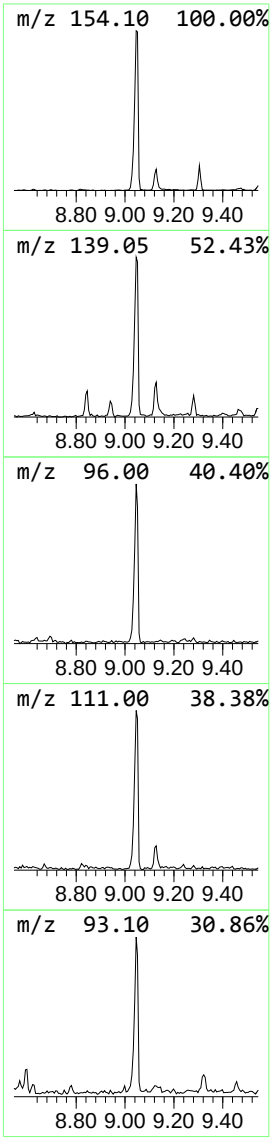
****

Peak Number 7 Phenol, 2,6-dimethoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.045	96.49 ng	1292090	Acenaphthene-d10	9.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,6-dimethoxy-	154	C8H10O3	000091-10-1	97
2	Phenol, 3,4-dimethoxy-	154	C8H10O3	002033-89-8	53
3	3-Amino-2,6-dimethoxypyridine	154	C7H10N2O2	028020-37-3	50
4	Formic acid, 2,6-dimethoxyphenyl...	182	C9H10O4	1000368-91-0	43
5	5-Fluoro-2-hydroxyacetophenone	154	C8H7FO2	000394-32-1	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061221\
Data File : BF124287.D
Acq On : 12 Jun 2021 15:37
Operator : JU/CG
Sample : M2674-01 5X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TMR-DS-01-060921

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

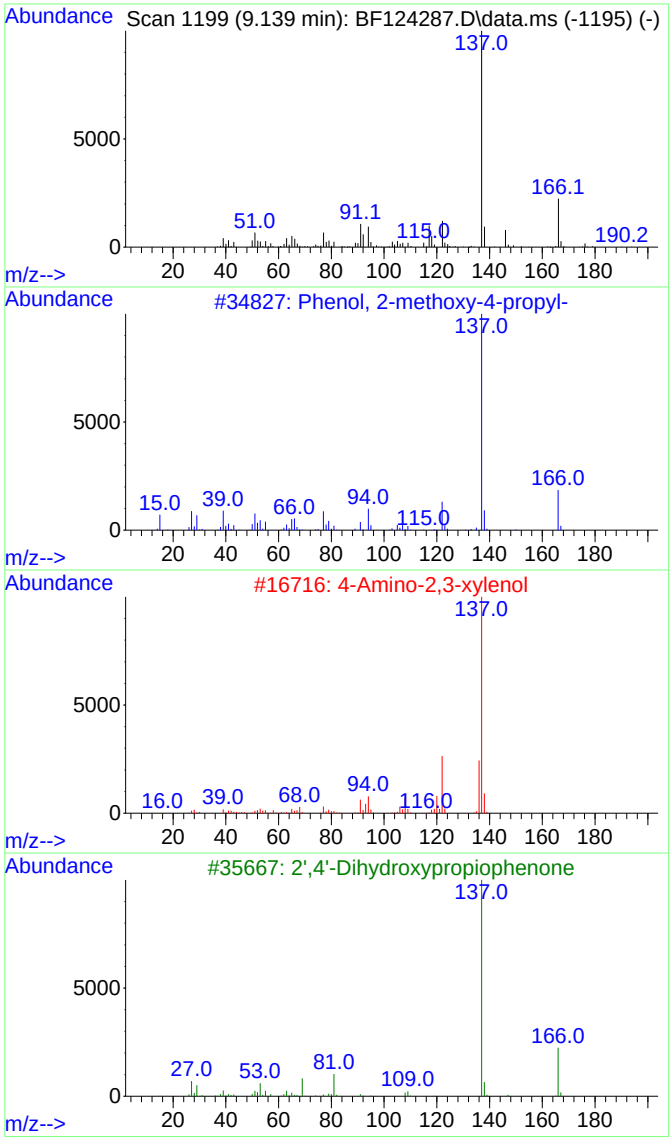
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

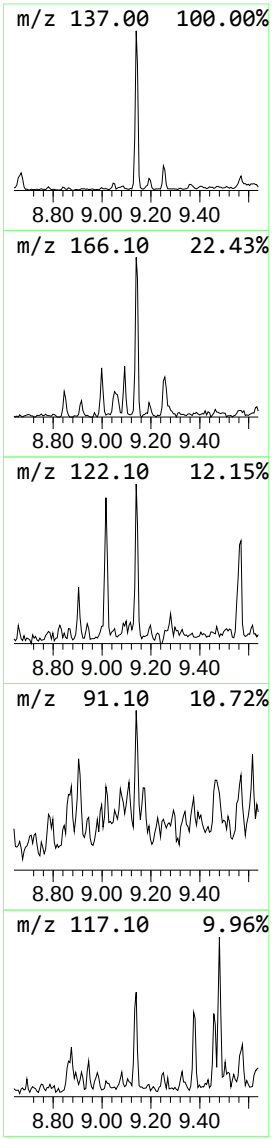
****

Peak Number 8 Phenol, 2-methoxy-4-propyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.139	55.96 ng	749354	Acenaphthene-d10	9.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-methoxy-4-propyl-	166	C10H14O2	002785-87-7	81
2	4-Amino-2,3-xylenol	137	C8H11NO	003096-69-3	52
3	2',4'-Dihydroxypropiophenone	166	C9H10O3	005792-36-9	52
4	Homovanillyl alcohol	168	C9H12O3	002380-78-1	50
5	Phenol, 3-(dimethylamino)-	137	C8H11NO	000099-07-0	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061221\
Data File : BF124287.D
Acq On : 12 Jun 2021 15:37
Operator : JU/CG
Sample : M2674-01 5X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TMR-DS-01-060921

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

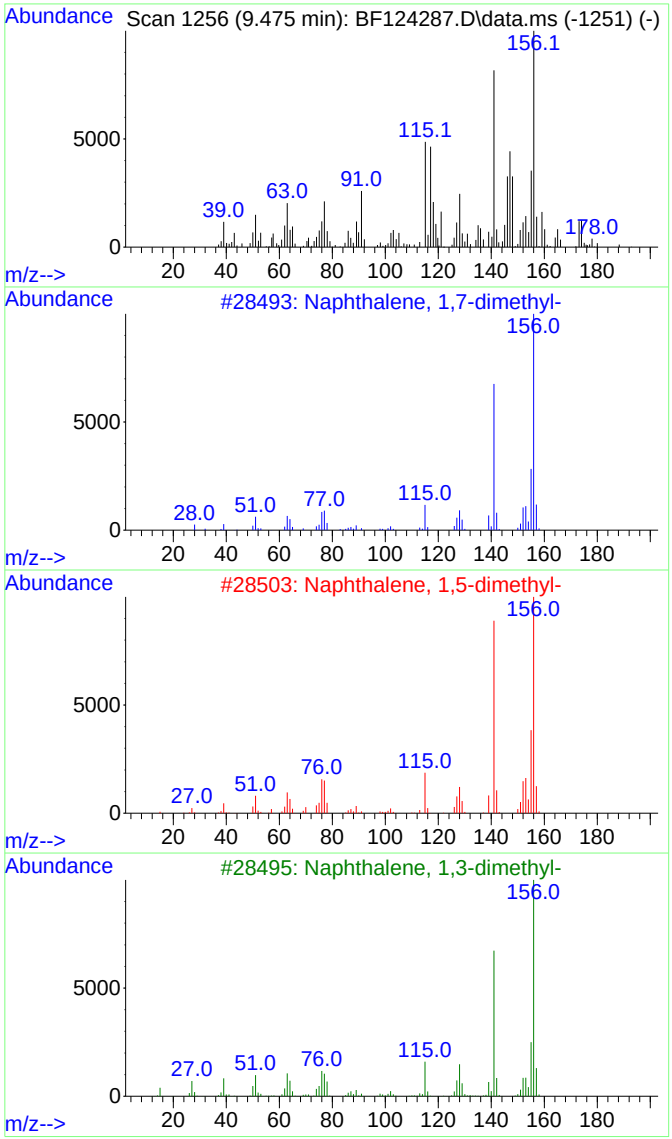
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

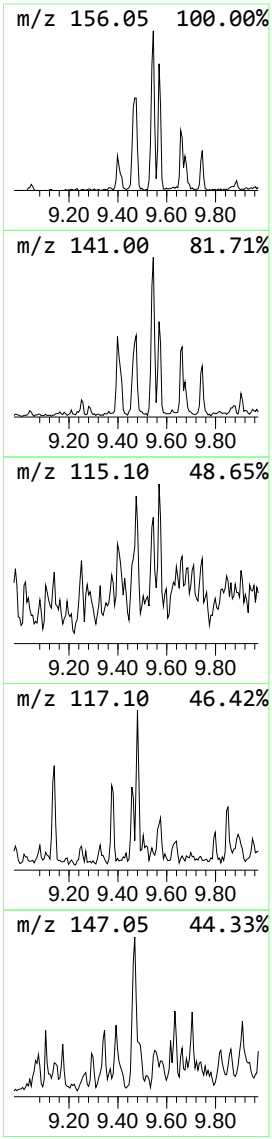
****

Peak Number 9 Naphthalene, 1,7-dimethyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.475	57.38 ng	768452	Acenaphthene-d10	9.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	89
2	Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	89
3	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	89
4	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	89
5	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061221\
Data File : BF124287.D
Acq On : 12 Jun 2021 15:37
Operator : JU/CG
Sample : M2674-01 5X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TMR-DS-01-060921

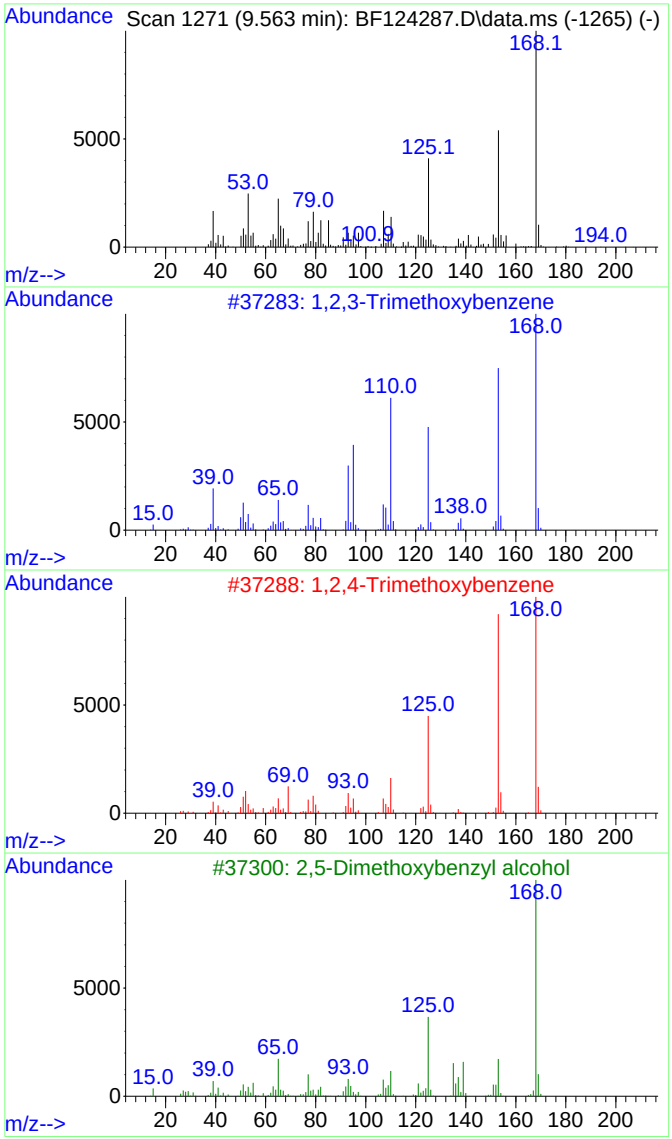
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

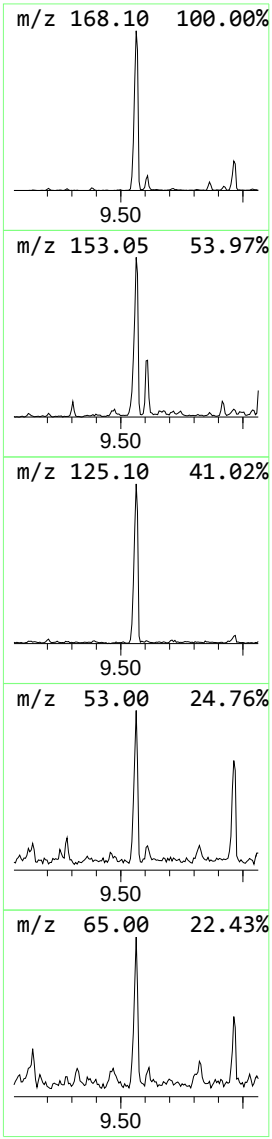
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1,2,3-Trimethoxybenzene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.563	174.02 ng	2330310	Acenaphthene-d10	9.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,3-Trimethoxybenzene	168	C9H12O3	000634-36-6	76
2	1,2,4-Trimethoxybenzene	168	C9H12O3	000135-77-3	62
3	2,5-Dimethoxybenzyl alcohol	168	C9H12O3	033524-31-1	60
4	4-Methoxy-2,2,5-trimethylcyclope...	168	C9H12O3	1000185-67-3	59
5	Dehydroacetic Acid	168	C8H8O4	000520-45-6	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061221\
Data File : BF124287.D
Acq On : 12 Jun 2021 15:37
Operator : JU/CG
Sample : M2674-01 5X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TMR-DS-01-060921

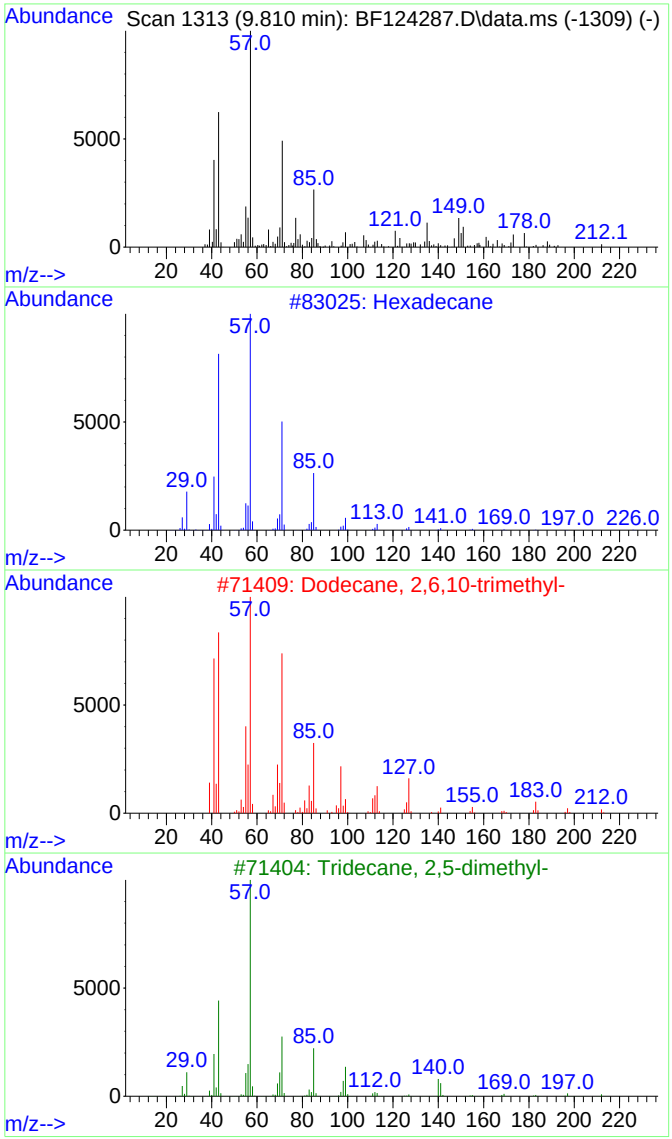
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

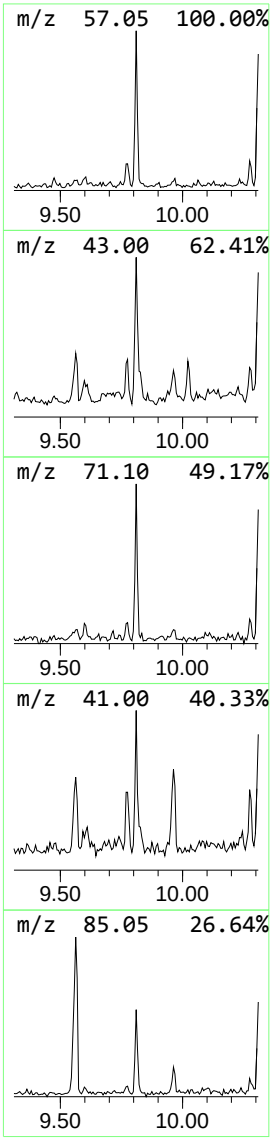
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 unknown9.810 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.810	39.62 ng	530517	Acenaphthene-d10	9.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	49
2	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	46
3	Tridecane, 2,5-dimethyl-	212	C15H32	056292-66-1	43
4	Decane, 1-bromo-2-methyl-	234	C11H23Br	127839-47-8	43
5	Tetradecane	198	C14H30	000629-59-4	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061221\
Data File : BF124287.D
Acq On : 12 Jun 2021 15:37
Operator : JU/CG
Sample : M2674-01 5X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TMR-DS-01-060921

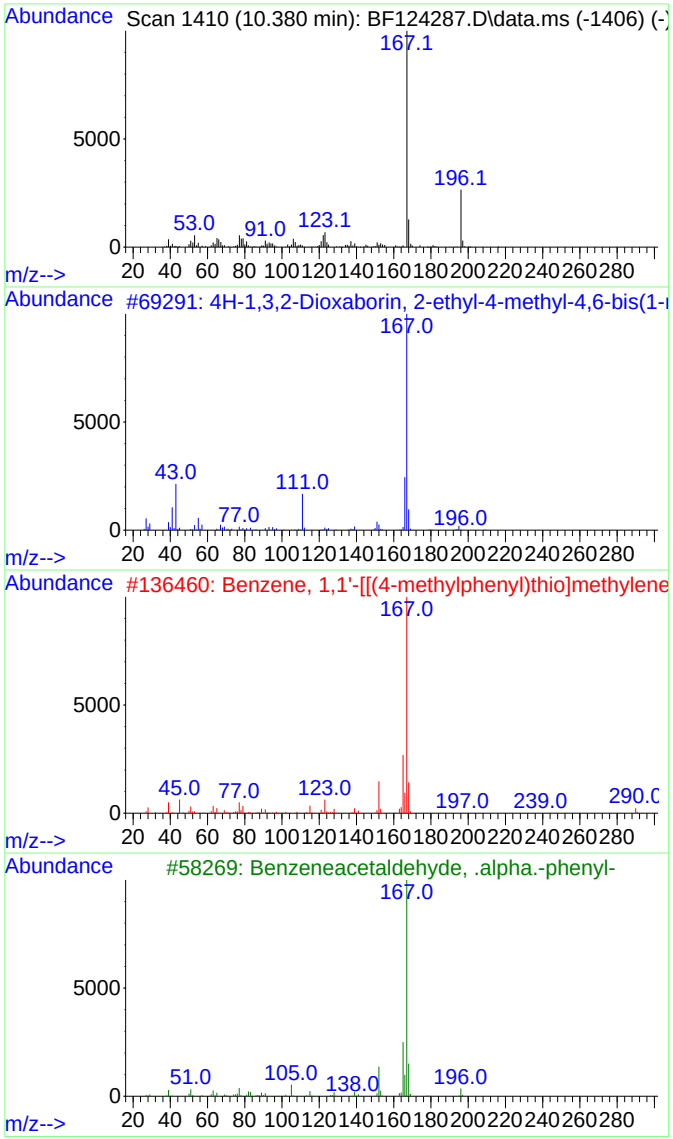
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

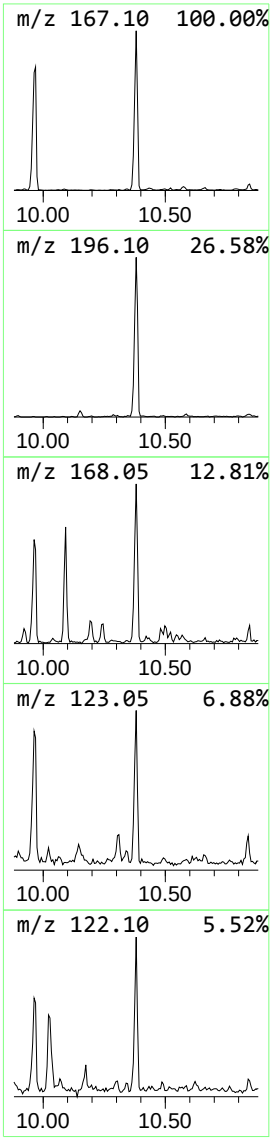
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 4H-1,3,2-Dioxaborin, 2-ethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.380	112.49 ng	1506400	Acenaphthene-d10	9.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-1,3,2-Dioxaborin, 2-ethyl-4-m...	210	C12H23BO2	074421-11-7	50
2	Benzene, 1,1'-[[(4-methylphenyl)...	290	C20H18S	032110-49-9	42
3	Benzeneacetaldehyde, .alpha.-phe...	196	C14H12O	000947-91-1	40
4	2-Propanone, 1,1-diphenyl-	210	C15H14O	000781-35-1	40
5	Benzene, 1,1'-propylidenebis-	196	C15H16	001530-03-6	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061221\
Data File : BF124287.D
Acq On : 12 Jun 2021 15:37
Operator : JU/CG
Sample : M2674-01 5X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TMR-DS-01-060921

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

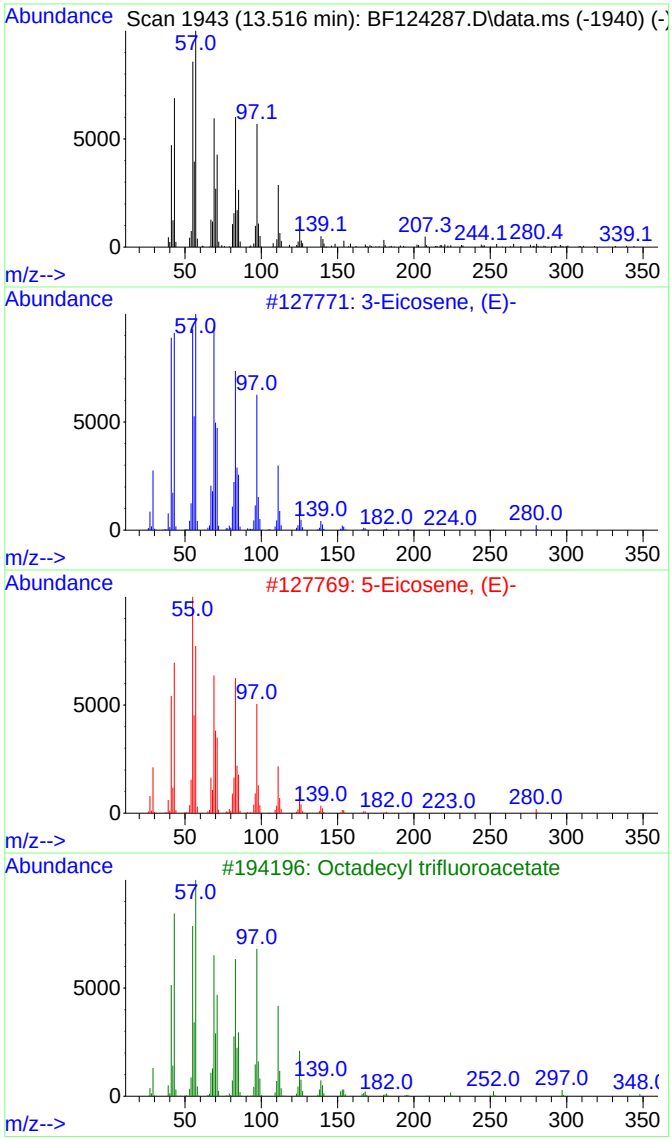
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

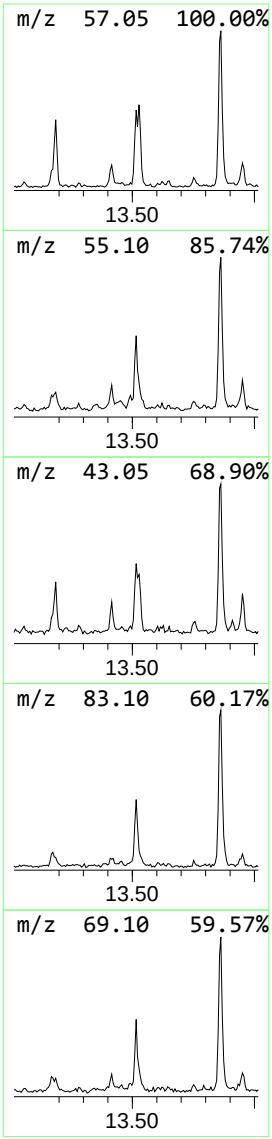
****

Peak Number 13 3-Eicosene, (E)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.515	69.50 ng	893435	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	95
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	93
3	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
4	1-Heptacosanol	396	C27H56O	002004-39-9	91
5	1-Tricosene	322	C23H46	018835-32-0	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061221\
Data File : BF124287.D
Acq On : 12 Jun 2021 15:37
Operator : JU/CG
Sample : M2674-01 5X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TMR-DS-01-060921

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

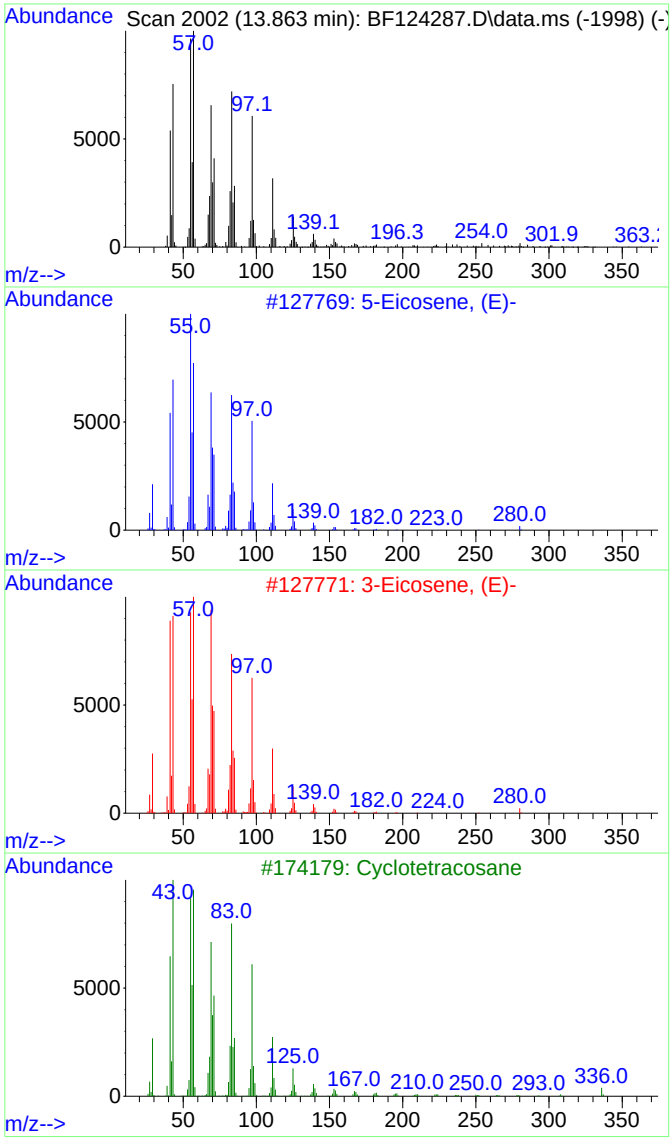
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

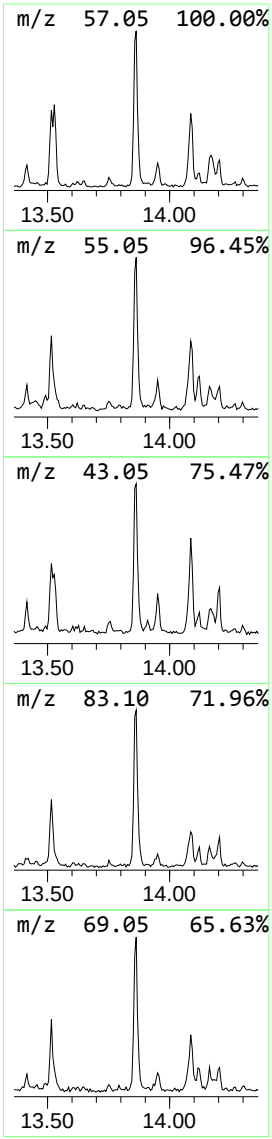
****

Peak Number 14 5-Eicosene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.863	131.67 ng	1692690	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	97
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	96
3	Cyclotetracosane	336	C24H48	000297-03-0	95
4	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	94
5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061221\
Data File : BF124287.D
Acq On : 12 Jun 2021 15:37
Operator : JU/CG
Sample : M2674-01 5X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TMR-DS-01-060921

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

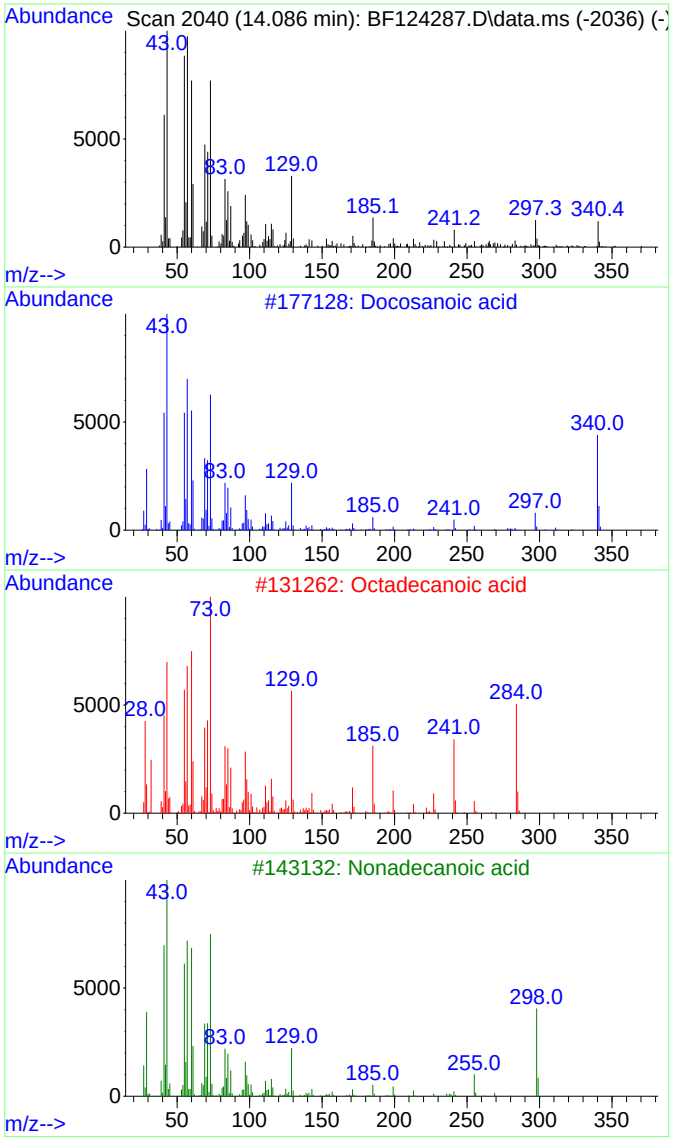
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

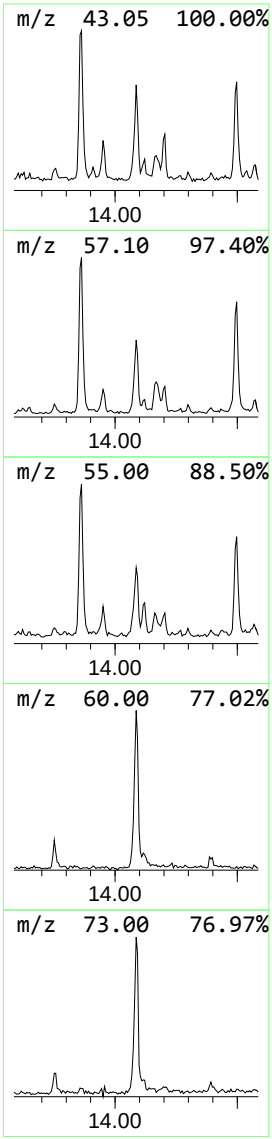
****

Peak Number 15 Docosanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.086	83.70 ng	1075960	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosanoic acid	340	C22H44O2	000112-85-6	99
2	Octadecanoic acid	284	C18H36O2	000057-11-4	95
3	Nonadecanoic acid	298	C19H38O2	000646-30-0	93
4	n-Decanoic acid	172	C10H20O2	000334-48-5	62
5	Tridecanoic acid	214	C13H26O2	000638-53-9	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061221\
Data File : BF124287.D
Acq On : 12 Jun 2021 15:37
Operator : JU/CG
Sample : M2674-01 5X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TMR-DS-01-060921

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

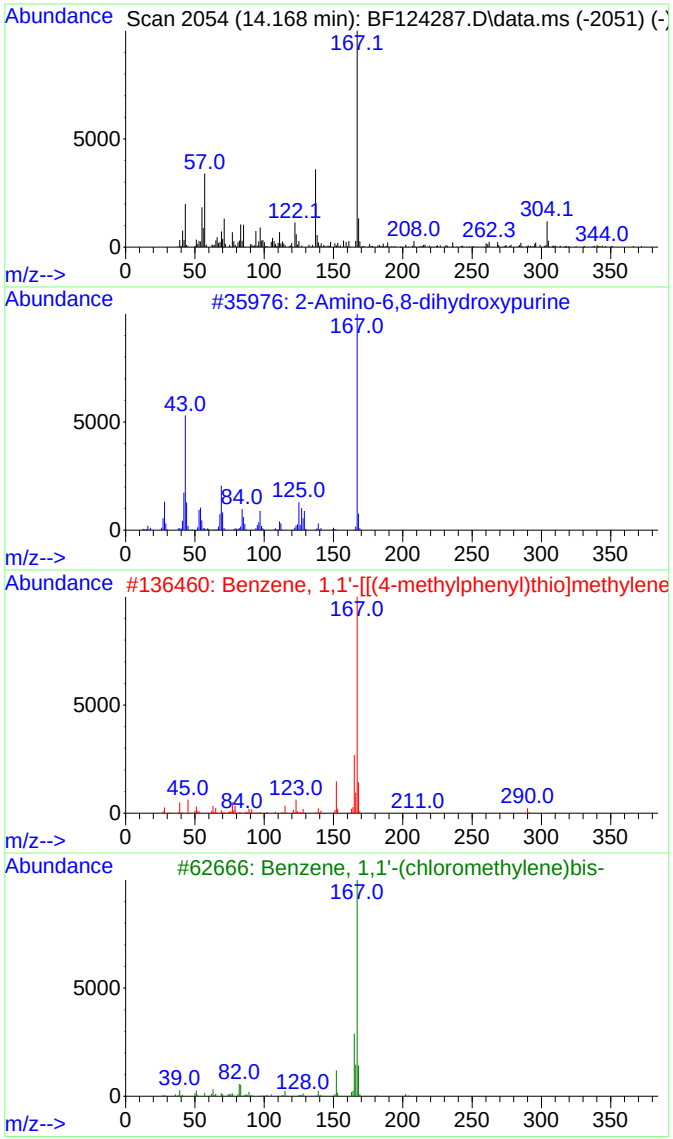
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

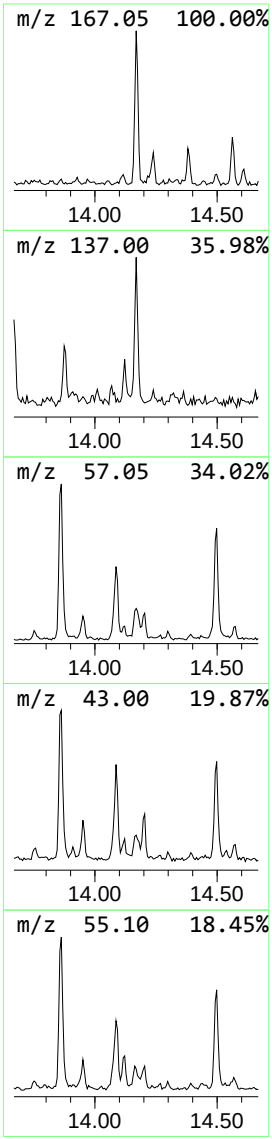
****

Peak Number 16 2-Amino-6,8-dihydroxypurine Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.168	43.88 ng	564078	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Amino-6,8-dihydroxypurine	167	C5H5N5O2	005614-64-2	53
2	Benzene, 1,1'-[[(4-methylphenyl)...	290	C20H18S	032110-49-9	43
3	Benzene, 1,1'-(chloromethylene)bis-	202	C13H11Cl	000090-99-3	43
4	2-Mercaptobenzothiazole	167	C7H5NS2	000149-30-4	43
5	Diethyl (4-biphenylylmethyl)phos...	304	C17H21O3P	030818-70-3	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061221\
Data File : BF124287.D
Acq On : 12 Jun 2021 15:37
Operator : JU/CG
Sample : M2674-01 5X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TMR-DS-01-060921

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

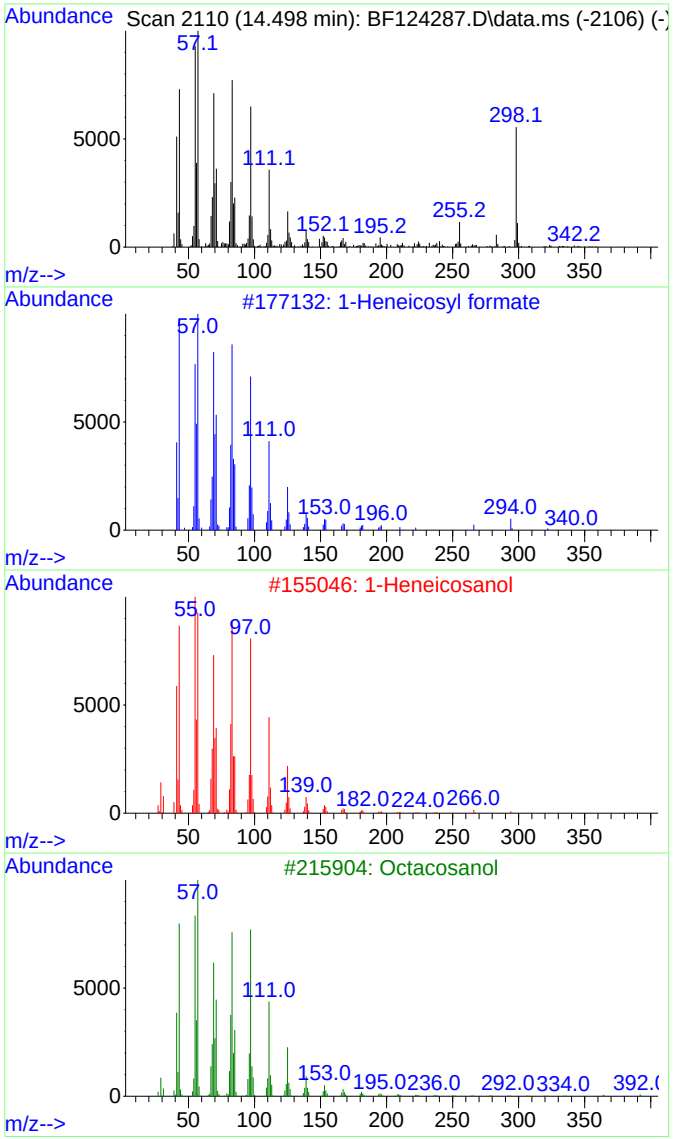
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

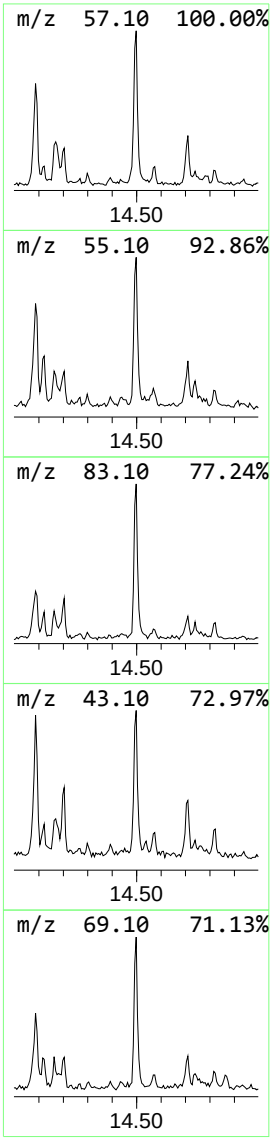
****

Peak Number 17 1-Heneicosyl formate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.498	104.04 ng	1337500	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	93
2	1-Heneicosanol	312	C21H44O	015594-90-8	90
3	Octacosanol	410	C28H58O	000557-61-9	90
4	1-Octadecanol	270	C18H38O	000112-92-5	89
5	13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061221\
Data File : BF124287.D
Acq On : 12 Jun 2021 15:37
Operator : JU/CG
Sample : M2674-01 5X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TMR-DS-01-060921

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

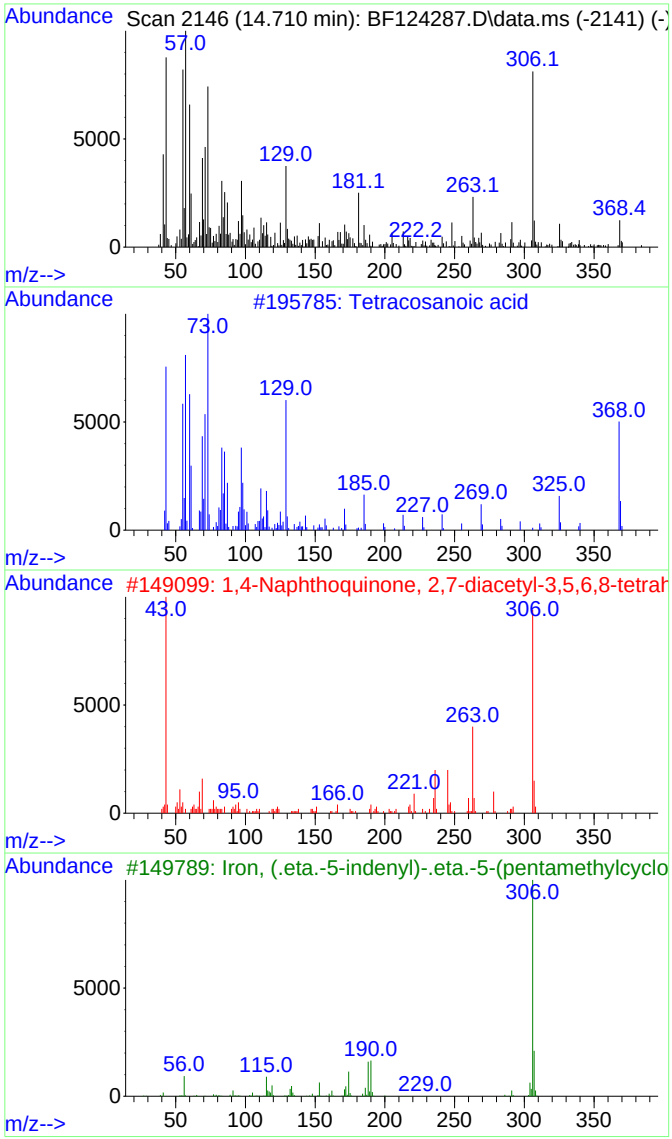
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

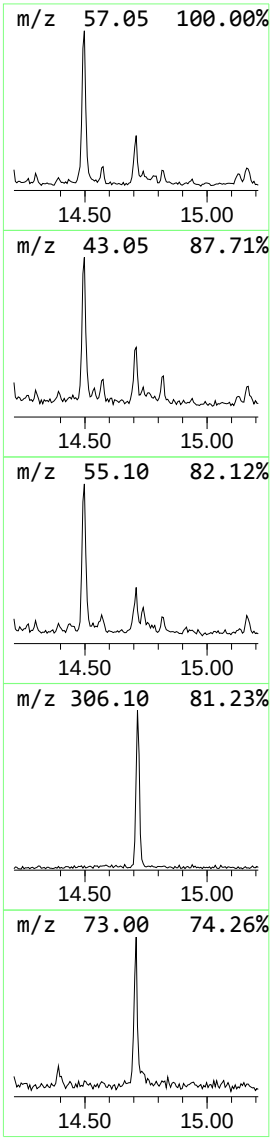
****

Peak Number 18 Tetracosanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.710	58.42 ng	750980	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosanoic acid	368	C24H48O2	000557-59-5	93
2	1,4-Naphthoquinone, 2,7-diacetyl...	306	C14H10O8	003404-89-5	38
3	Iron, (.eta.-5-indenyl)-.eta.-5-...	306	C19H22Fe	1000161-63-0	38
4	Carbazolo[3,4-a]carbazole, 5,8-d...	306	C22H14N2	007259-12-3	27
5	[5-(3-Nitro-phenyl)-furan-2-ylme...	306	C18H14N2O3	330567-57-2	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061221\
Data File : BF124287.D
Acq On : 12 Jun 2021 15:37
Operator : JU/CG
Sample : M2674-01 5X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TMR-DS-01-060921

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

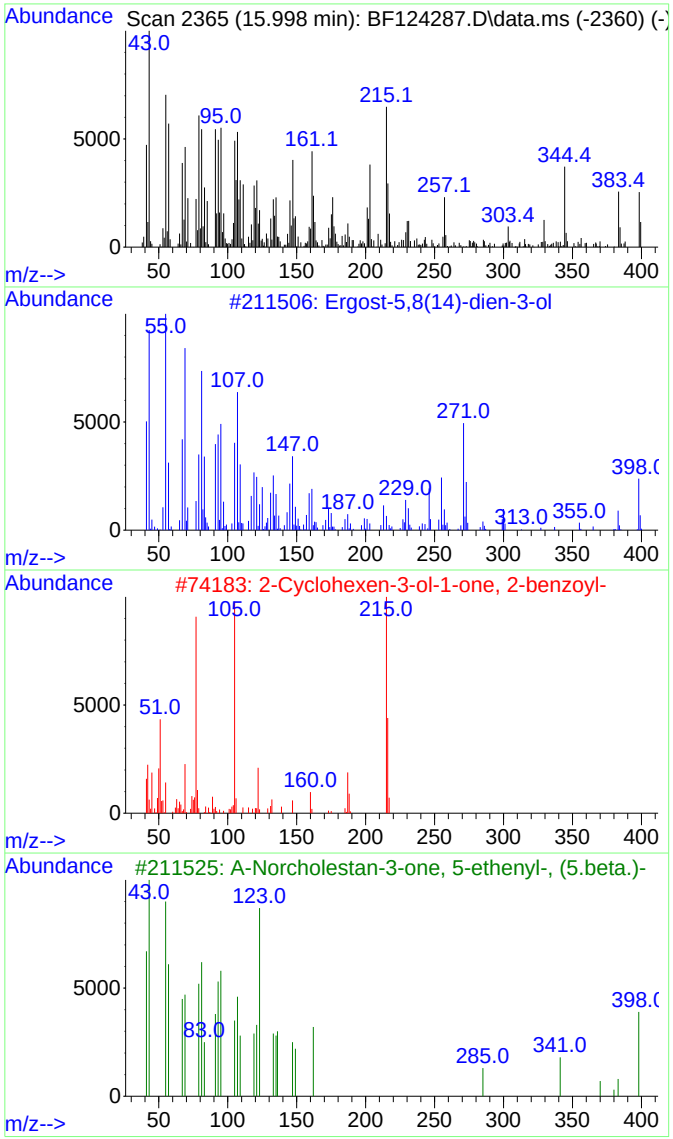
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

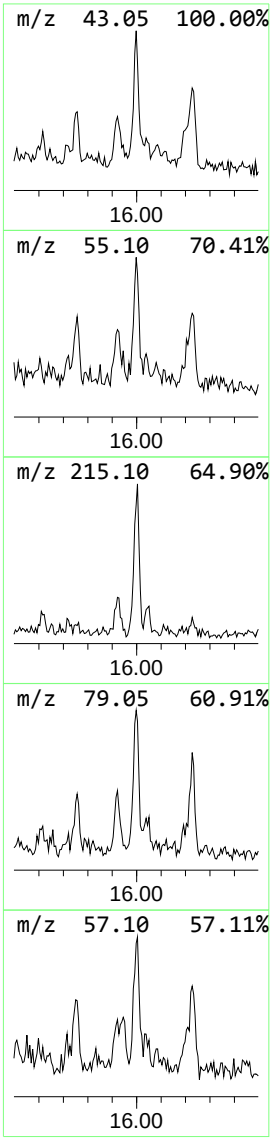
****

Peak Number 19 unknown15.998 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.998	44.17 ng	836206	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ergost-5,8(14)-dien-3-ol	398	C28H46O	177962-83-3	46
2	2-Cyclohexen-3-ol-1-one, 2-benzoyl-	216	C13H12O3	061834-43-3	44
3	A-Norcholestan-3-one, 5-ethenyl-...	398	C28H46O	019594-90-2	35
4	7,22-Ergostadienol	398	C28H46O	1000253-06-7	25
5	5,6-Dihydro-3a-ergosterol	398	C28H46O	1000253-60-4	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061221\
Data File : BF124287.D
Acq On : 12 Jun 2021 15:37
Operator : JU/CG
Sample : M2674-01 5X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TMR-DS-01-060921

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

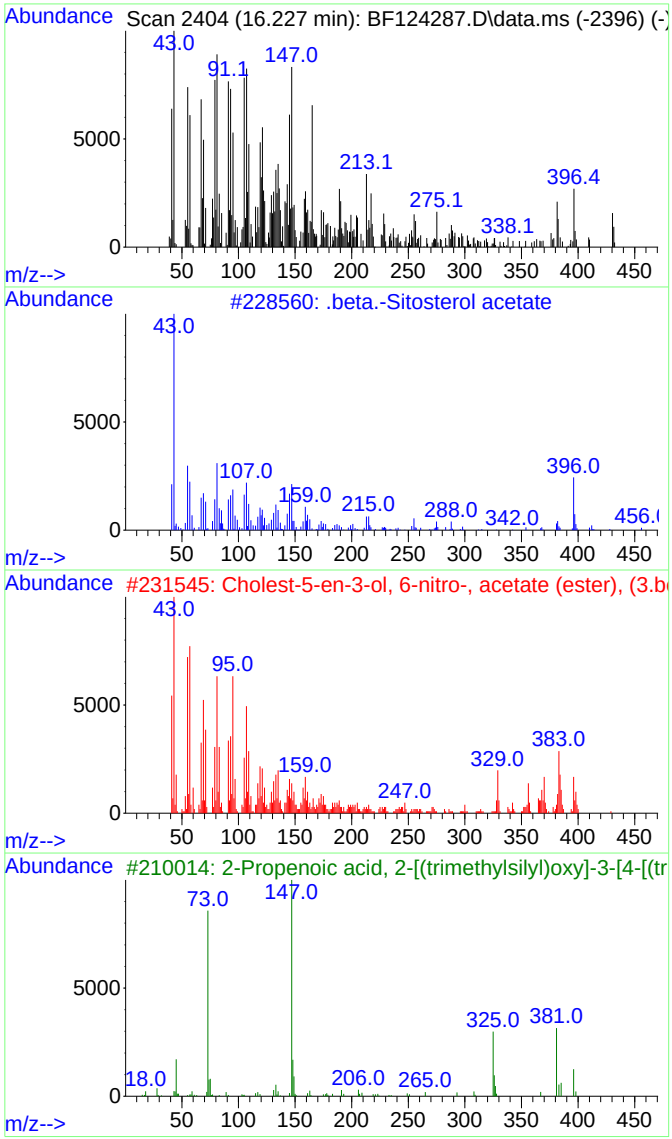
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

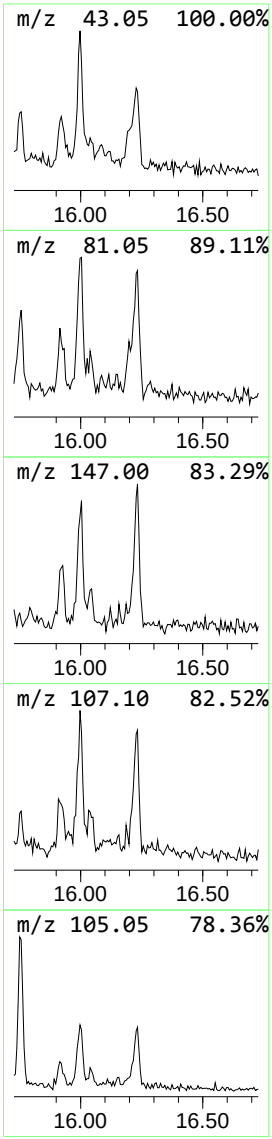
****

Peak Number 20 unknown16.227 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.227	56.75 ng	1074370	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	25
2	Cholest-5-en-3-ol, 6-nitro-, ace...	473	C29H47NO4	001912-54-5	17
3	2-Propenoic acid, 2-[(trimethyls...	396	C18H32O4Si3	027750-74-9	9
4	D-Homo-5.alpha.-androstan-17a-on...	382	C25H34O3	017429-43-5	9
5	p-Toluenesulfonyl-tyrosyl-S-carb...	552	C25H32N2O8S2	097191-78-1	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061221\
Data File : BF124287.D
Acq On : 12 Jun 2021 15:37
Operator : JU/CG
Sample : M2674-01 5X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TMR-DS-01-060921

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
Benzofuran, 7-m...	7.534	56.6	ng	506747	2	8.128	178933	20.0
Benzofuran, 2-m...	7.575	62.9	ng	562438	2	8.128	178933	20.0
Phenol, 2,3-dim...	7.992	59.7	ng	534060	2	8.128	178933	20.0
1H-Benzimidazol...	8.298	99.7	ng	891796	2	8.128	178933	20.0
Phenol, 3-ethyl...	8.492	73.3	ng	655391	2	8.128	178933	20.0
Phenol, 4-ethyl...	8.628	98.6	ng	882051	2	8.128	178933	20.0
Phenol, 2,6-dim...	9.045	96.5	ng	1292090	3	9.886	267827	20.0
Phenol, 2-metho...	9.139	56.0	ng	749354	3	9.886	267827	20.0
Naphthalene, 1,...	9.475	57.4	ng	768452	3	9.886	267827	20.0
1,2,3-Trimethox...	9.563	174.0	ng	2330310	3	9.886	267827	20.0
unknown9.810	9.810	39.6	ng	530517	3	9.886	267827	20.0
4H-1,3,2-Dioxab...	10.380	112.5	ng	1506400	3	9.886	267827	20.0
3-Eicosene, (E)-	13.515	69.5	ng	893435	5	14.027	257111	20.0
5-Eicosene, (E)-	13.863	131.7	ng	1692690	5	14.027	257111	20.0
Docosanoic acid	14.086	83.7	ng	1075960	5	14.027	257111	20.0
2-Amino-6,8-dih...	14.168	43.9	ng	564078	5	14.027	257111	20.0
1-Heneicosyl fo...	14.498	104.0	ng	1337500	5	14.027	257111	20.0
Tetracosanoic acid	14.710	58.4	ng	750980	5	14.027	257111	20.0
unknown15.998	15.998	44.2	ng	836206	6	15.515	378650	20.0
unknown16.227	16.227	56.8	ng	1074370	6	15.515	378650	20.0