LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091520\
Data File : BF121580.D
Acq On : 15 Sep 2020 16:30
Operator : JU/CG
Sample : L4007-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11929

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-BF091020.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	4	8	24	rVB	255127	422140	4.53%	0.372%
2	4.428	392	398	404	rBV	1654829	1854437	19.90%	1.636%
3	4.487	404	408	419	rVB	188550	216313	2.32%	0.191%
4	5.063	498	506	509	rBV	2711914	3991608	42.83%	3.521%
5	5.457	569	573	580	rBV	2285178	2002239	21.48%	1.766%
6	6.469	741	745	754	rBV	3598387	3556155	38.16%	3.137%
7	6.828	803	806	813	rVB	1463546	1345710	14.44%	1.187%
8	7.392	894	902	905	rBV	2879304	2797628	30.02%	2.468%
9	7.428	905	908	912	rVB	221918	190712	2.05%	0.168%
10	8.116	1018	1025	1028	rBV2	1970331	2185391	23.45%	1.928%
11	8.175	1032	1035	1038	rVB	144996	128565	1.38%	0.113%
12	8.404	1067	1074	1081	rBV5	115834	239360	2.57%	0.211%
13	8.492	1086	1089	1093	rBV2	120576	128468	1.38%	0.113%
14	8.533	1093	1096	1099	rBV	255534	230661	2.47%	0.203%
15	8.704	1121	1125	1129	rBV	952717	751273	8.06%	0.663%
16	8.827	1143	1146	1148	rVB	216331	181568	1.95%	0.160%
17	8.880	1148	1155	1158	rBV4	198519	203283	2.18%	0.179%
18	8.922	1159	1162	1166	rVB	148847	128807	1.38%	0.114%
19	8.986	1171	1173	1175	rBV2	119690	113085	1.21%	0.100%
20	9.069	1184	1187	1190	rVB	168377	150091	1.61%	0.132%
21	9.110	1191	1194	1196	rBV	147944	124066	1.33%	0.109%
22	9.133	1196	1198	1202	rVB	339919	281746	3.02%	0.249%
23	9.192	1202	1208	1211	rBV	5114067	4716901	50.61%	4.161%
24	9.269	1217	1221	1226	rBV	1402427	1192124	12.79%	1.052%
25	9.386	1238	1241	1245	rVB	139813	147627	1.58%	0.130%
26	9.451	1248	1252	1256	rVV	1149900	999306	10.72%	0.882%
27	9.527	1261	1265	1267	rVV	391663	429187	4.60%	0.379%
28	9.551	1267	1269	1271	rVV2	278169	224898	2.41%	0.198%
29	9.586	1271	1275	1278	rVV2	522316	772270	8.29%	0.681%
30	9.610	1278	1279	1282	rVB2	206540	134459	1.44%	0.119%
31	9.645	1282	1285	1288	rBV2	198137	209273	2.25%	0.185%
32	9.798	1308	1311	1316	rVB	1558090	1259511	13.51%	1.111%
33	9.869	1319	1323	1325	rVB	2393457	1905199	20.44%	1.681%
34	9.974	1337	1341	1345	rVB3	169871	244475	2.62%	0.216%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091520\
Data File : BF121580.D
Acq On : 15 Sep 2020 16:30
Operator : JU/CG
Sample : L4007-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11929

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-BF091020.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	10.027	1345	1350	1353	rBV3	136257	242041	2.60%	0.214%
36	10.063	1353	1356	1359	rVV2	258293	342699	3.68%	0.302%
37	10.122	1362	1366	1370	rVV3	284008	448936	4.82%	0.396%
38	10.180	1374	1376	1379	rVV	240451	212624	2.28%	0.188%
39	10.298	1388	1396	1399	rVV	1718778	1560437	16.74%	1.376%
40	10.345	1399	1404	1411	rVB8	118651	314845	3.38%	0.278%
41	10.416	1411	1416	1421	rBV4	171605	297181	3.19%	0.262%
42	10.522	1428	1434	1436	rBV	535225	629963	6.76%	0.556%
43	10.569	1439	1442	1445	rVB2	135718	144413	1.55%	0.127%
44	10.604	1445	1448	1451	rBV2	134399	127408	1.37%	0.112%
45	10.651	1451	1456	1460	rVB2	782900	857742	9.20%	0.757%
46	10.769	1473	1476	1482	rBV	1513582	2069138	22.20%	1.825%
47	10.963	1504	1509	1511	rBV4	142011	181435	1.95%	0.160%
48	11.221	1549	1553	1555	rBV	1144363	1034938	11.10%	0.913%
49	11.251	1555	1558	1564	rVB	532915	582807	6.25%	0.514%
50	11.351	1571	1575	1578	rBV	2280516	2018102	21.65%	1.780%
51	11.398	1580	1583	1587	rVB4	83794	133620	1.43%	0.118%
52	11.527	1602	1605	1608	rVB	178141	160100	1.72%	0.141%
53	11.598	1614	1617	1622	rBV	162794	190454	2.04%	0.168%
54	11.645	1622	1625	1628	rBV	1039047	850331	9.12%	0.750%
55	11.757	1638	1644	1647	rVB	8387982	9320208	100.00%	8.222%
56	11.810	1650	1653	1658	rBV2	111762	134750	1.45%	0.119%
57	11.880	1662	1665	1667	rBV	309209	289387	3.10%	0.255%
58	12.051	1691	1694	1698	rVV	770767	598122	6.42%	0.528%
59	12.104	1700	1703	1708	rVB3	109107	117415	1.26%	0.104%
60	12.151	1708	1711	1713	rBV	271179	239444	2.57%	0.211%
61	12.433	1755	1759	1761	rBV	3726286	4221972	45.30%	3.724%
62	12.457	1761	1763	1770	rVB	5759302	5597317	60.06%	4.938%
63	12.545	1773	1778	1781	rVB	7178970	7017238	75.29%	6.190%
64	12.757	1811	1814	1816	rBV	224903	187503	2.01%	0.165%
65	12.810	1821	1823	1833	rVB	312471	413688	4.44%	0.365%
66	12.939	1840	1845	1848	rBV	5038742	4821952	51.74%	4.254%
67	13.033	1859	1861	1864	rBV3	167939	147499	1.58%	0.130%
68	13.110	1869	1874	1876	rBV2	643298	944090	10.13%	0.833%
69	13.139	1876	1879	1882	rVV4	384684	578107	6.20%	0.510%
70	13.192	1882	1888	1897	rVB2	2731566	3767993	40.43%	3.324%
71	13.262	1897	1900	1902	rBV	1037846	891425	9.56%	0.786%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091520\
Data File : BF121580.D
Acq On : 15 Sep 2020 16:30
Operator : JU/CG
Sample : L4007-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11929

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-BF091020.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	13.292	1902	1905	1908	rVB2	194107	203308	2.18%	0.179%
73	13.374	1914	1919	1923	rVB	5062478	5574142	59.81%	4.917%
74	13.421	1924	1927	1930	rVB2	209341	225721	2.42%	0.199%
75	13.468	1932	1935	1939	rBV	423862	449861	4.83%	0.397%
76	13.510	1939	1942	1948	rVB	325427	324058	3.48%	0.286%
77	13.574	1948	1953	1955	rBV2	711476	1035535	11.11%	0.913%
78	13.598	1955	1957	1959	rVV2	386174	377287	4.05%	0.333%
79	13.627	1959	1962	1967	rVV2	748329	1031990	11.07%	0.910%
80	13.680	1967	1971	1975	rVB3	409787	730549	7.84%	0.644%
81	13.715	1975	1977	1980	rVB	143569	124162	1.33%	0.110%
82	13.762	1980	1985	1987	rBV3	292877	499674	5.36%	0.441%
83	13.833	1994	1997	2006	rBV	975946	1219795	13.09%	1.076%
84	13.904	2006	2009	2011	rVV2	218603	271476	2.91%	0.239%
85	13.927	2011	2013	2017	rVB	855757	743598	7.98%	0.656%
86	13.986	2018	2023	2027	rBV	1654422	1570907	16.85%	1.386%
87	14.151	2048	2051	2059	rVB	195071	222210	2.38%	0.196%
88	14.457	2100	2103	2109	rVB3	170729	206357	2.21%	0.182%
89	14.545	2115	2118	2126	rVB	273103	264835	2.84%	0.234%
90	14.762	2152	2155	2158	rVB	151996	137177	1.47%	0.121%
91	15.098	2209	2212	2215	rBV	186376	182437	1.96%	0.161%
92	15.439	2266	2270	2274	rBV	988108	1202316	12.90%	1.061%
93	15.903	2346	2349	2354	rVB	97677	129007	1.38%	0.114%
94	15.962	2355	2359	2368	rVB2	123343	251439	2.70%	0.222%
95	16.139	2383	2389	2402	rBV	2262553	4399582	47.20%	3.881%
96	16.339	2416	2423	2428	rBV2	834775	1457009	15.63%	1.285%
97	16.392	2428	2432	2437	rVB3	146330	295563	3.17%	0.261%
98	16.939	2518	2525	2541	rVB	1568535	3294830	35.35%	2.906%
99	17.239	2569	2576	2589	rVB4	399394	1054895	11.32%	0.931%
100	18.321	2753	2760	2769	rVB3	286926	737487	7.91%	0.651%

Sum of corrected areas: 113363067

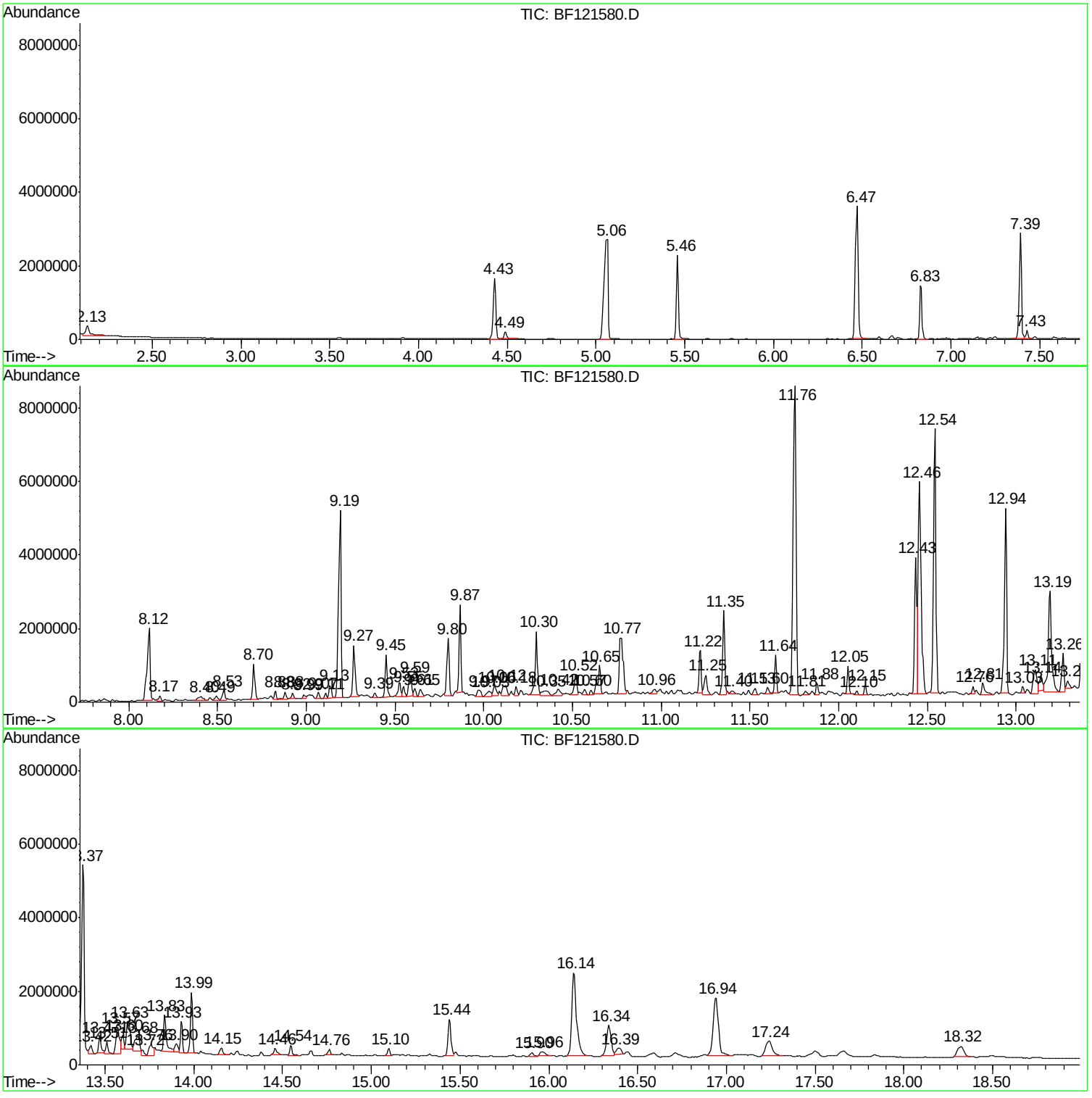
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091520\
Data File : BF121580.D
Acq On : 15 Sep 2020 16:30
Operator : JU/CG
Sample : L4007-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11929

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.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\BF091520\
Data File : BF121580.D
Acq On : 15 Sep 2020 16:30
Operator : JU/CG
Sample : L4007-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11929

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

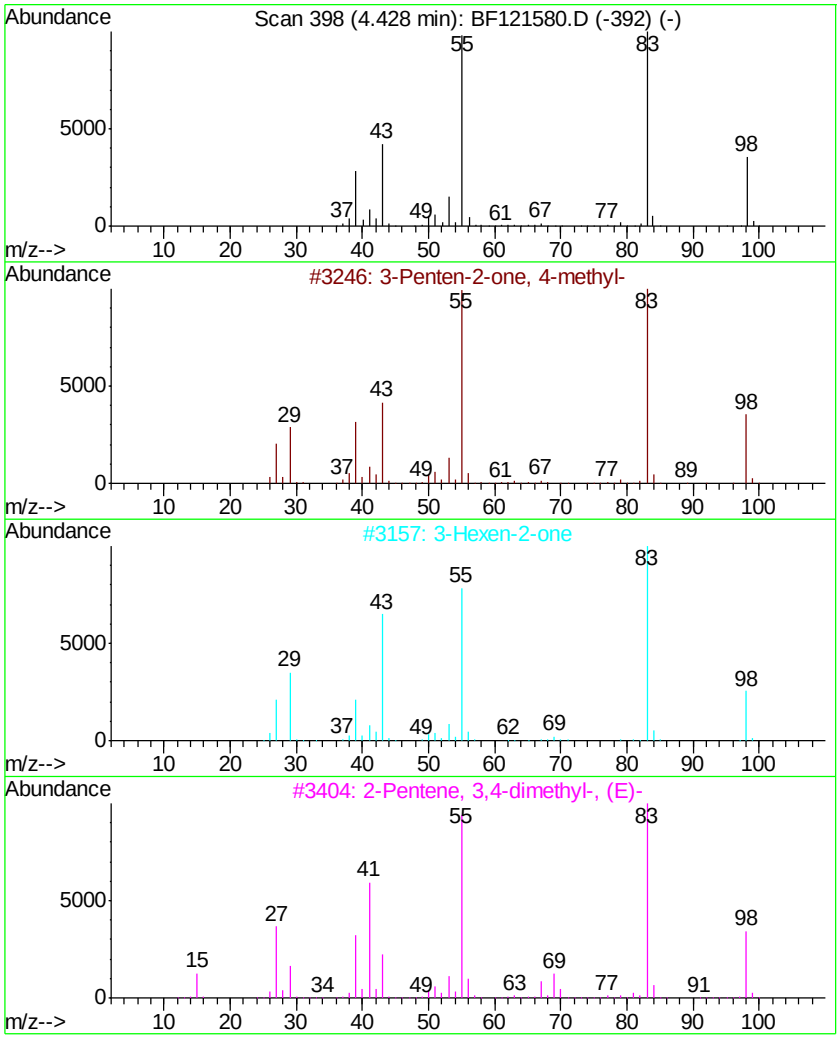
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

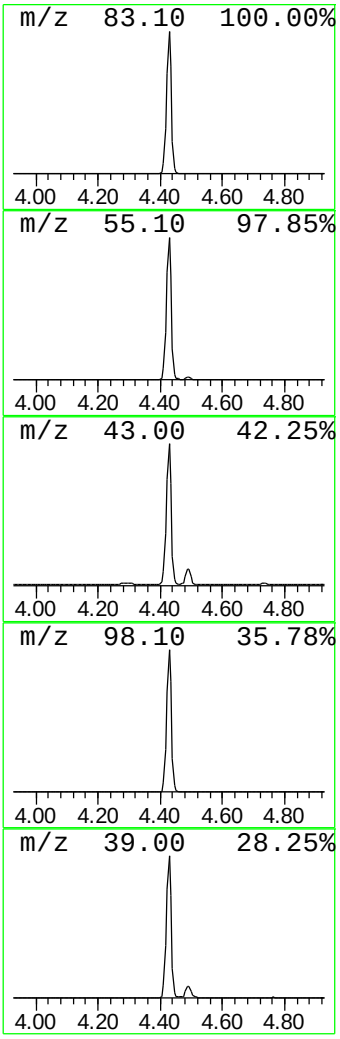
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.43	27.56 ng	1854440	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091520\
Data File : BF121580.D
Acq On : 15 Sep 2020 16:30
Operator : JU/CG
Sample : L4007-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11929

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

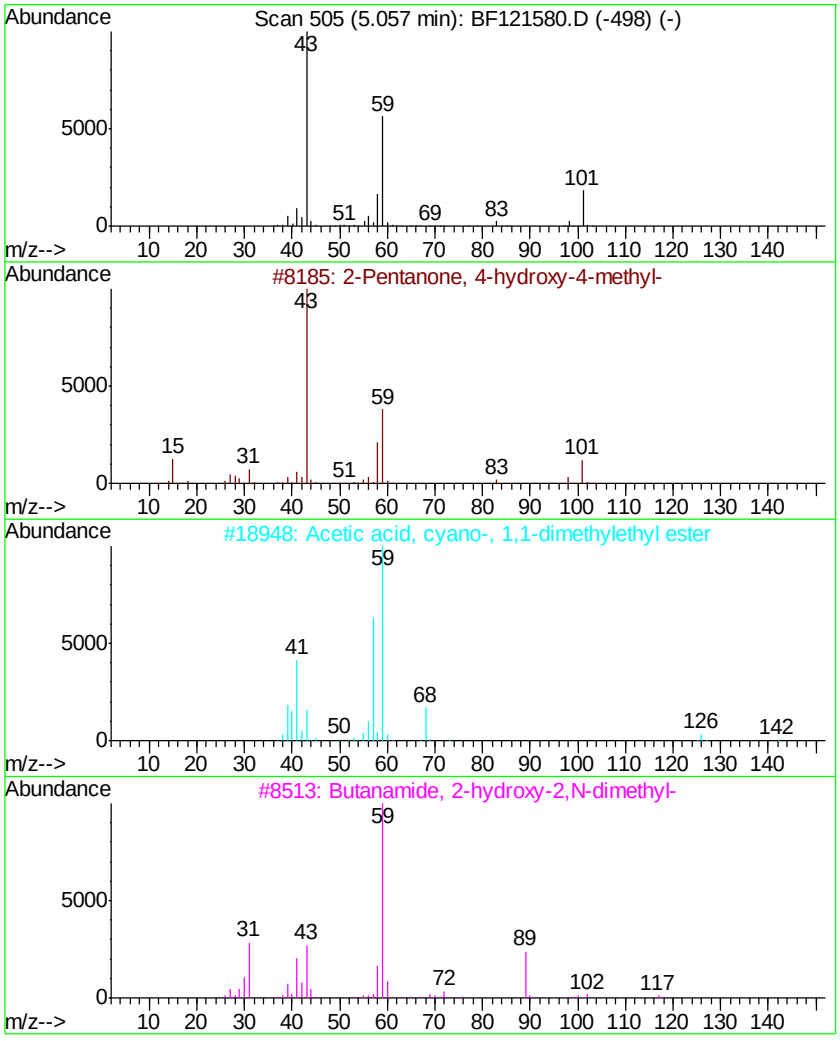
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

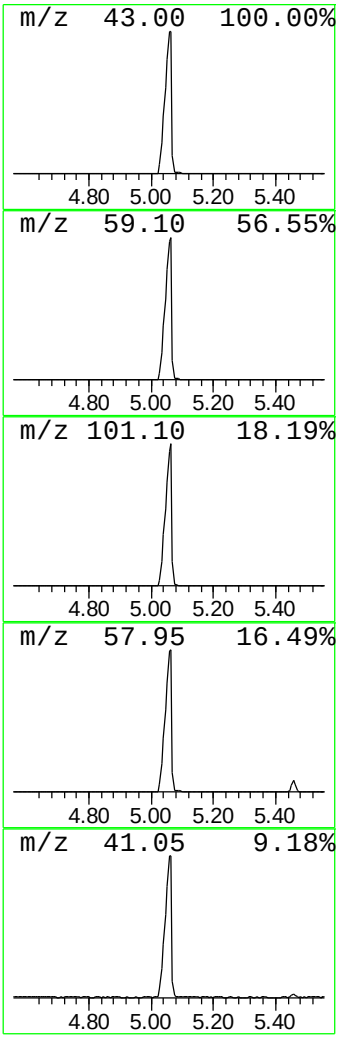
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	59.32 ng	3991610	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	Butanamide, 2-hydroxy-2,N-dimethyl-	117	C5H11NO2	039961-72-3	9
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091520\
Data File : BF121580.D
Acq On : 15 Sep 2020 16:30
Operator : JU/CG
Sample : L4007-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11929

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

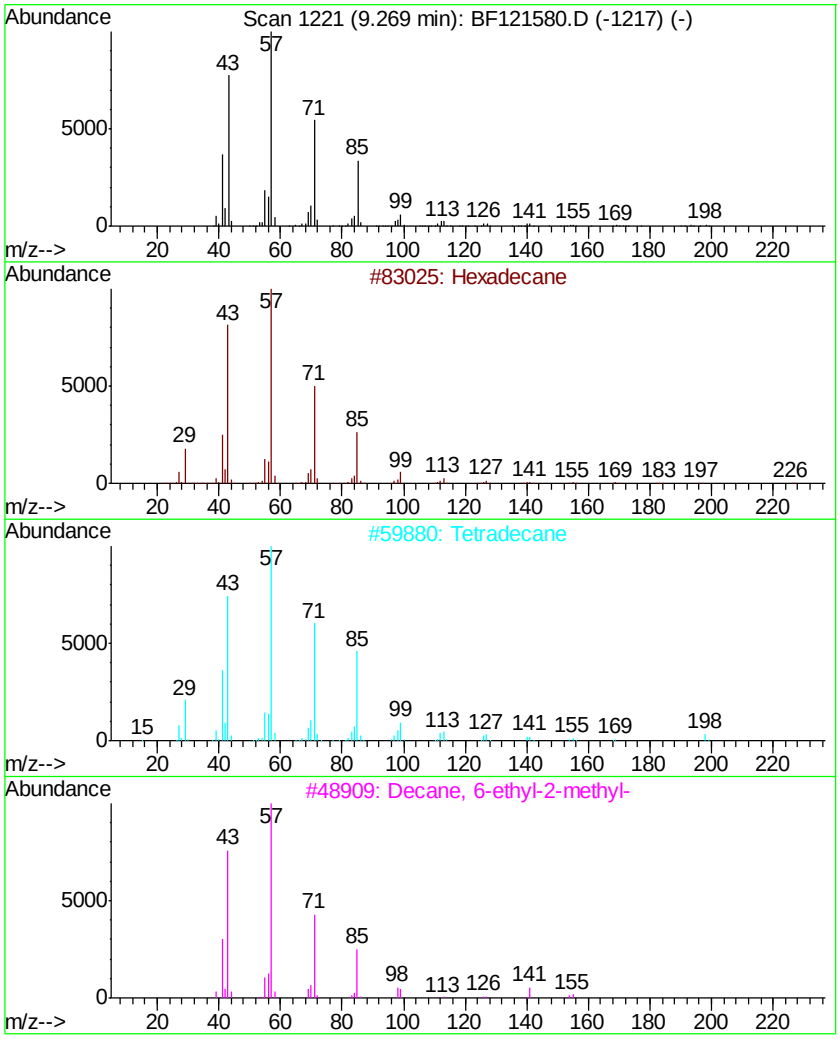
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

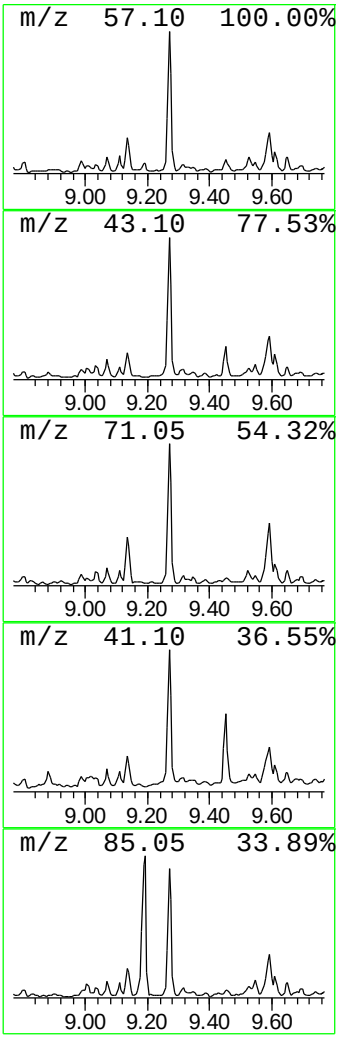
****

Peak Number 3 Hexadecane Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.27	12.51 ng	1192120	Acenaphthene-d10	9.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Tetradecane	198	C14H30	000629-59-4	90
3	Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	83
4	Decane, 3-bromo-	220	C10H21Br	030571-71-2	80
5	Tridecane, 6-methyl-	198	C14H30	013287-21-3	68





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091520\
Data File : BF121580.D
Acq On : 15 Sep 2020 16:30
Operator : JU/CG
Sample : L4007-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11929

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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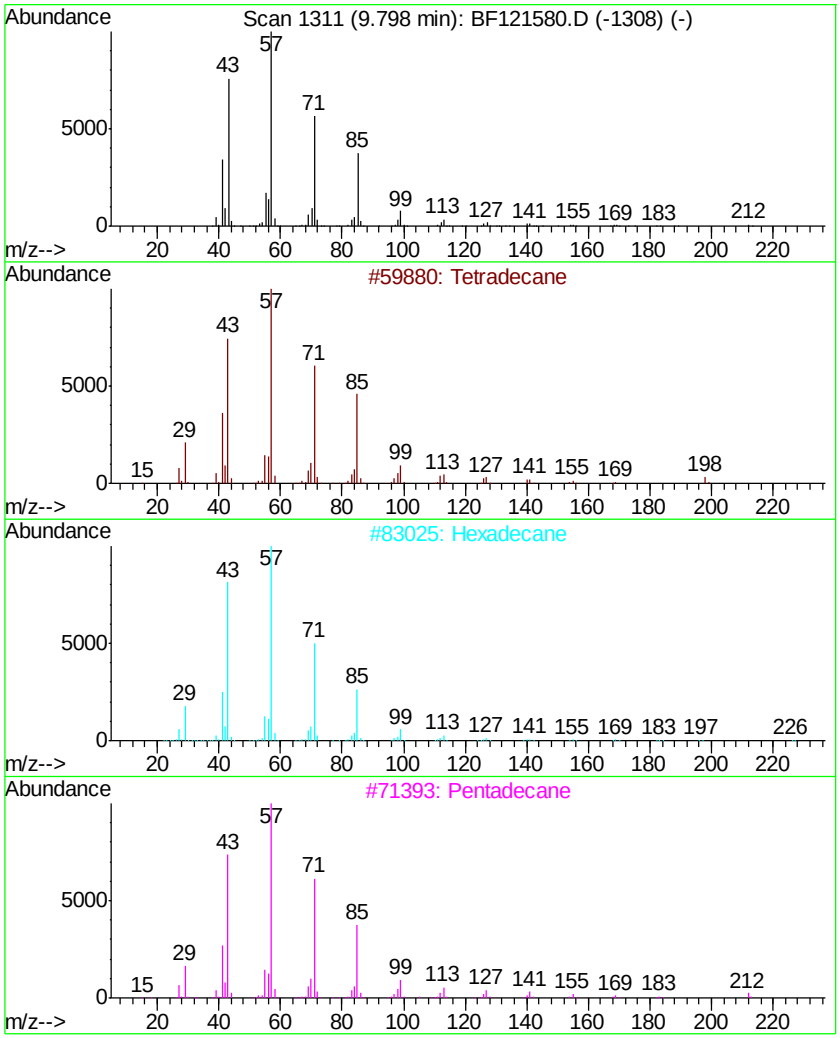
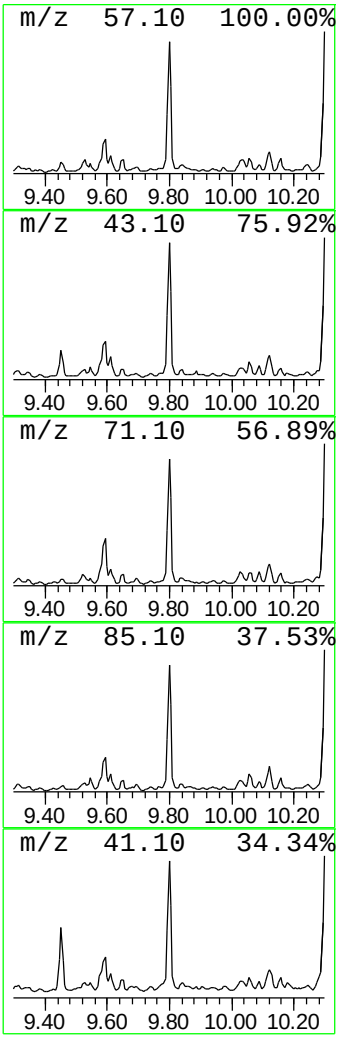
Peak Number 4 Tetradecane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.80	13.22 ng	1259510	Acenaphthene-d10	9.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	90
2	Hexadecane	226	C16H34	000544-76-3	90
3	Pentadecane	212	C15H32	000629-62-9	87
4	Tridecane	184	C13H28	000629-50-5	78
5	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	78





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091520\
Data File : BF121580.D
Acq On : 15 Sep 2020 16:30
Operator : JU/CG
Sample : L4007-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11929

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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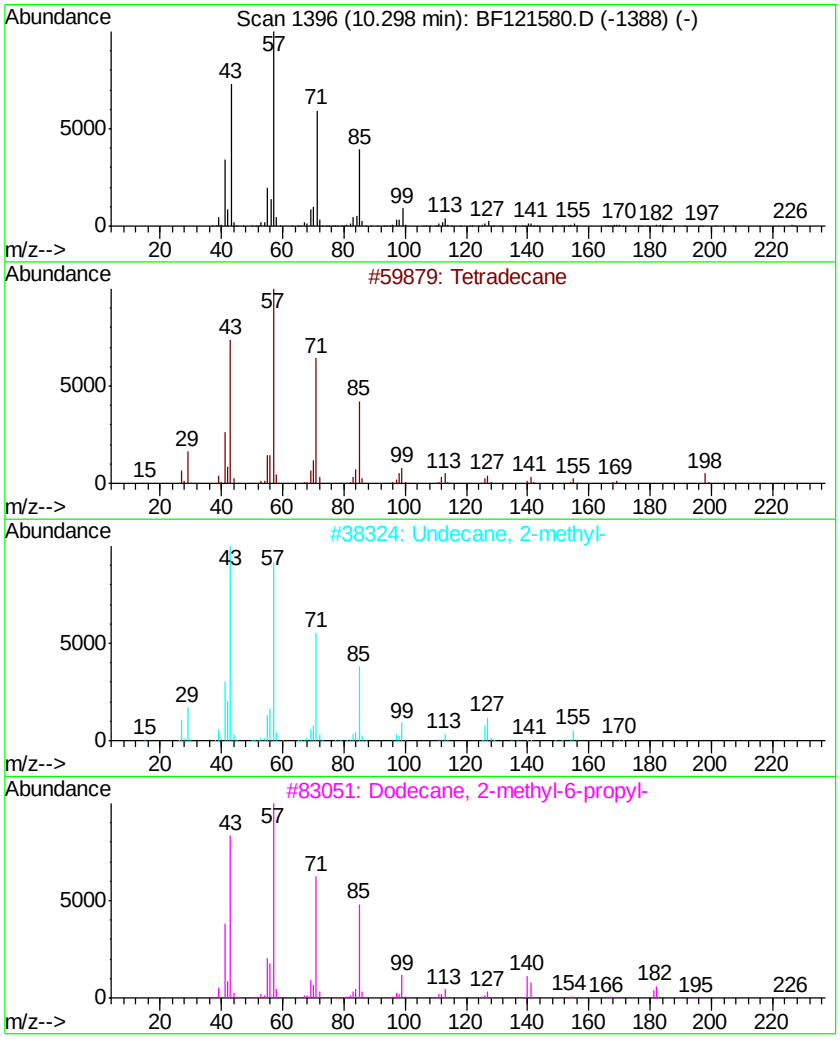
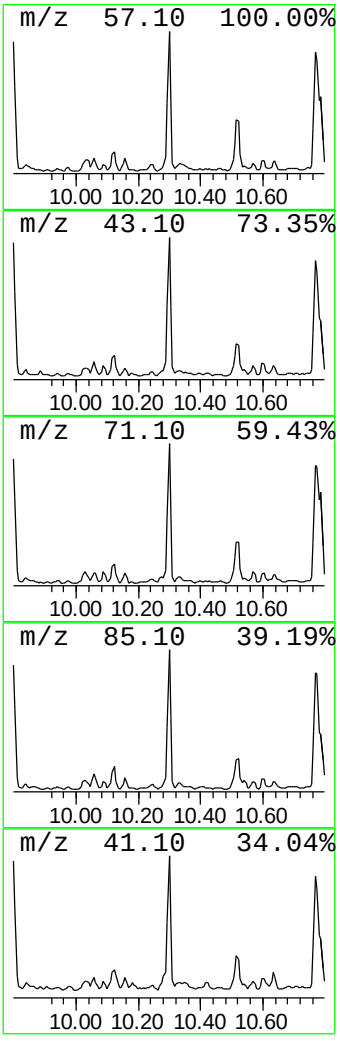
Peak Number 5 Undecane, 2-methyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.30	16.38 ng	1560440	Acenaphthene-d10	9.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	90
2	Undecane, 2-methyl-	170	C12H26	007045-71-8	87
3	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	86
4	Hexadecane	226	C16H34	000544-76-3	83
5	Tridecane	184	C13H28	000629-50-5	80





Library Search Compound Report

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Data File : BF121580.D
Acq On : 15 Sep 2020 16:30
Operator : JU/CG
Sample : L4007-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11929

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

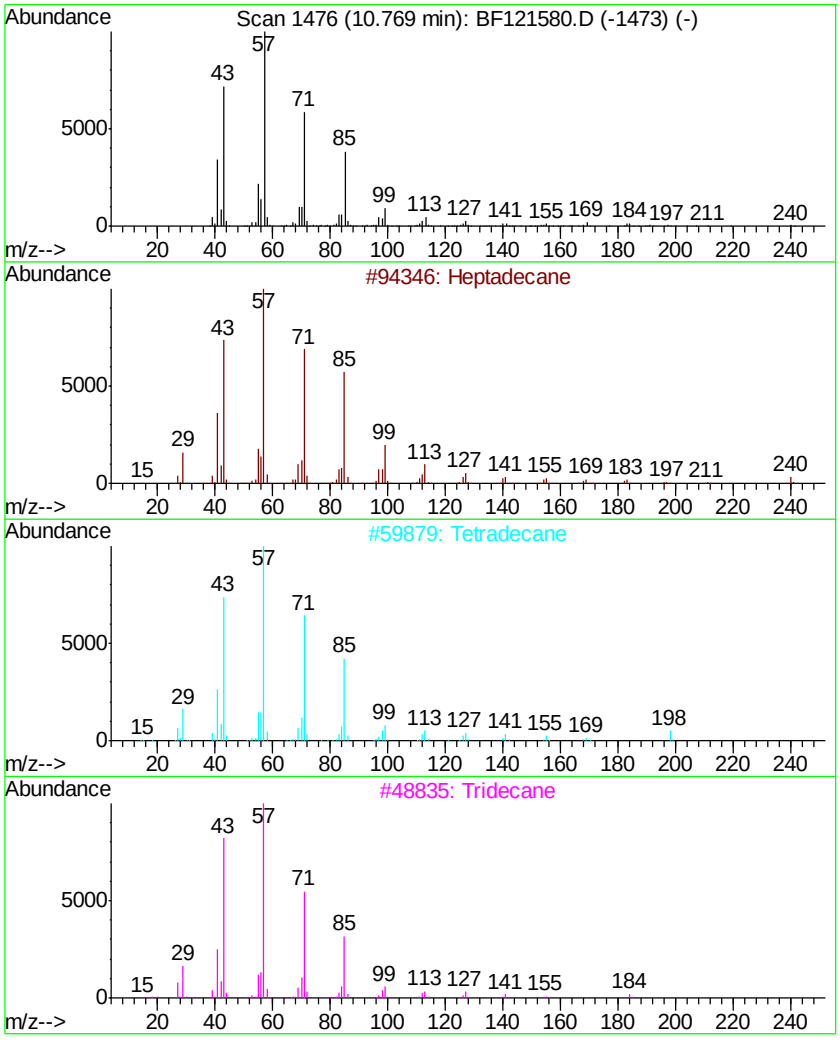
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

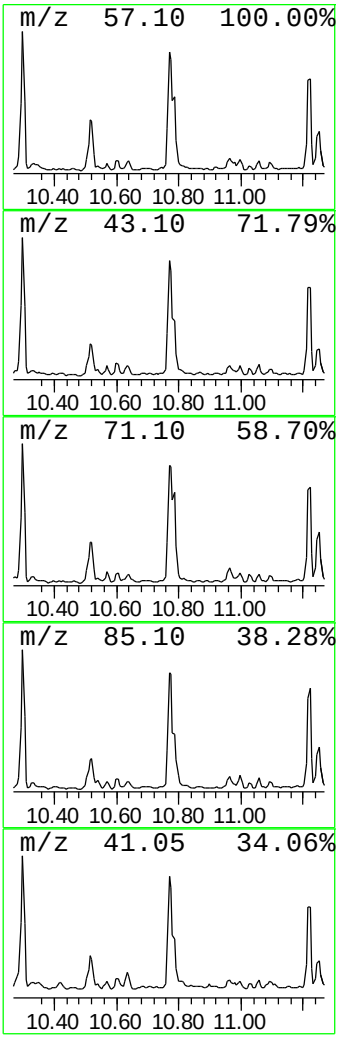
****

Peak Number 6 Heptadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.77	20.51 ng	2069140	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	97
2	Tetradecane	198	C14H30	000629-59-4	96
3	Tridecane	184	C13H28	000629-50-5	94
4	Tridecane, 6-propyl-	226	C16H34	055045-10-8	90
5	Nonadecane	268	C19H40	000629-92-5	86





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Sample : L4007-01
Misc :
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Instrument : BNA_F
ClientSampleId : 72-11929

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

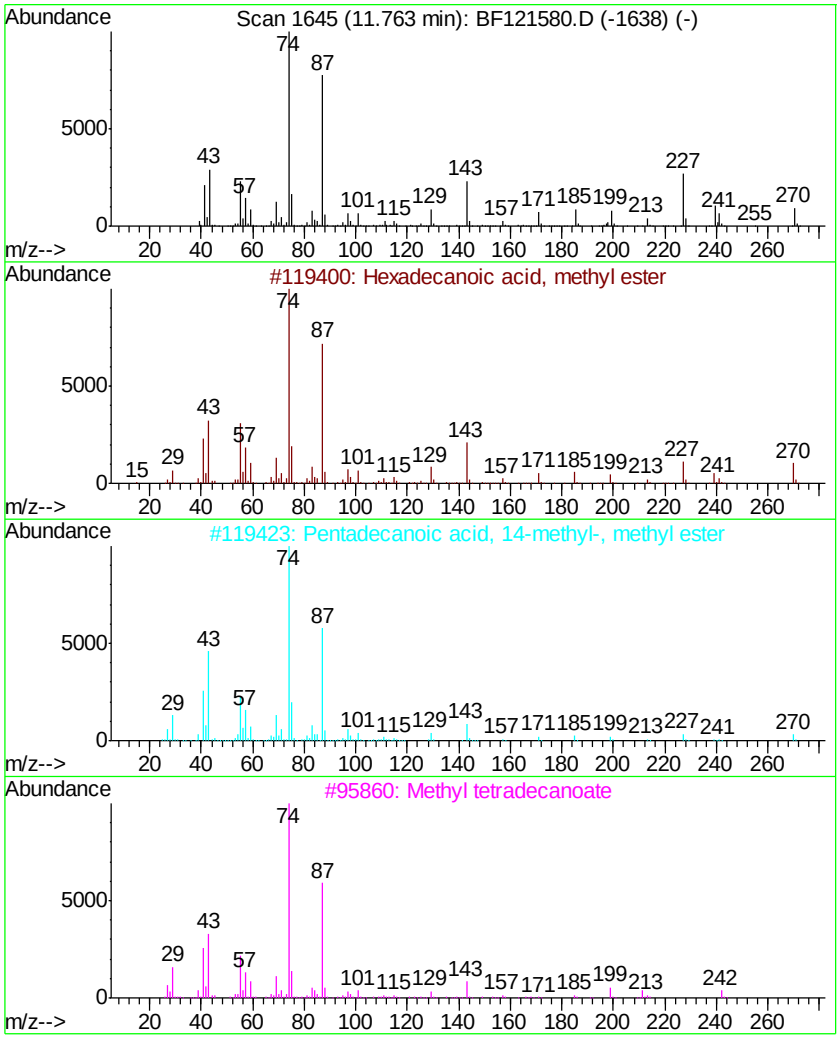
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

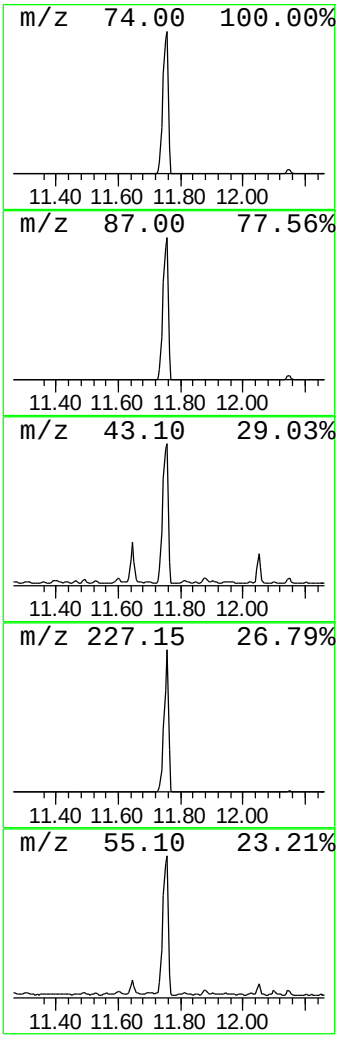
****

Peak Number 7 Hexadecanoic acid, methyl e... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.76	92.37 ng	9320210	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	95
3	Methyl tetradecanoate	242	C15H30O2	000124-10-7	91
4	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
5	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	87





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Operator : JU/CG
Sample : L4007-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11929

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

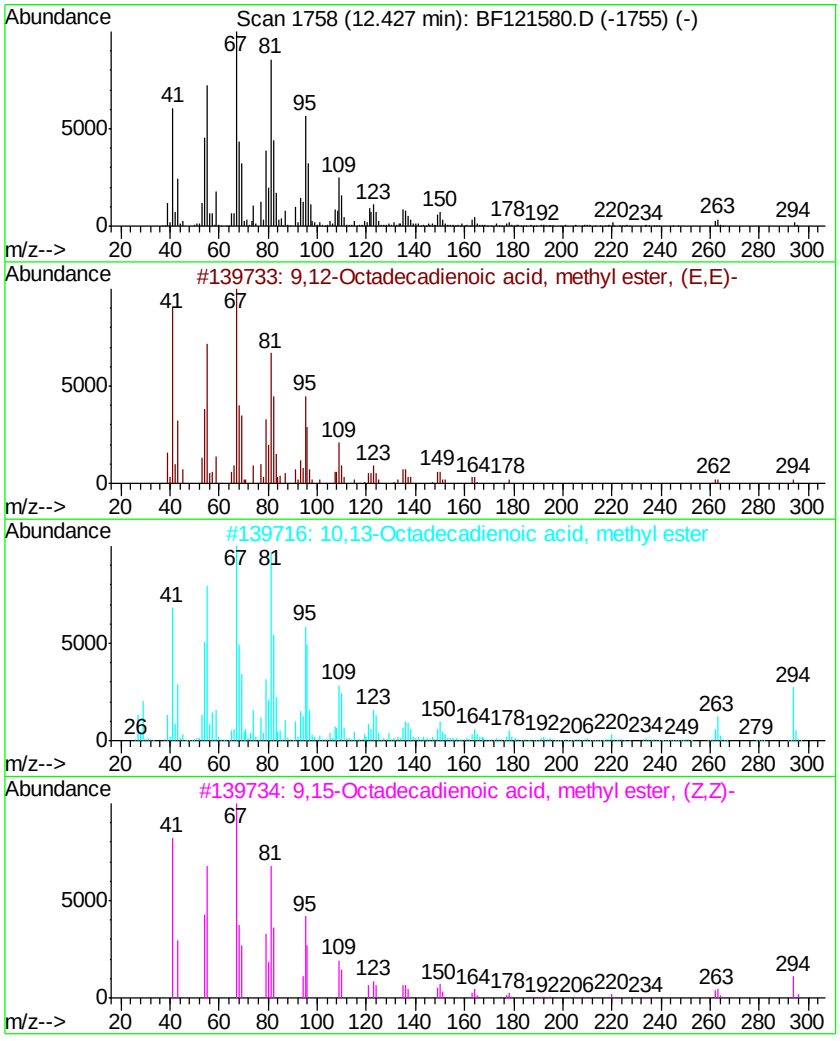
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

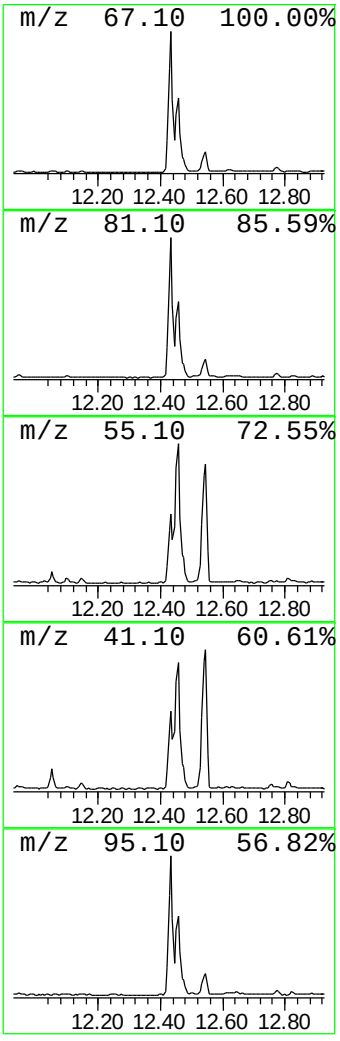
****

Peak Number 8 9,12-Octadecadienoic acid, ... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.43	41.84 ng	4221970	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
3	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
4	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
5	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99





Library Search Compound Report

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Acq On : 15 Sep 2020 16:30
Operator : JU/CG
Sample : L4007-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11929

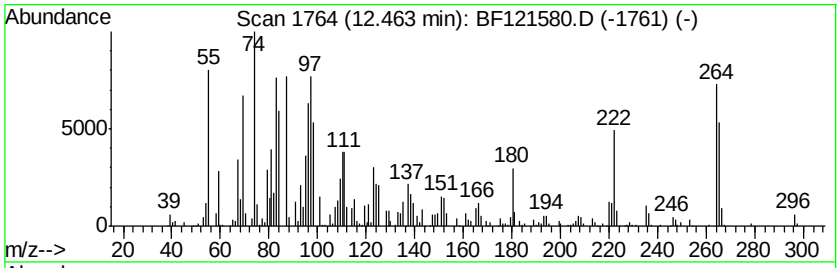
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

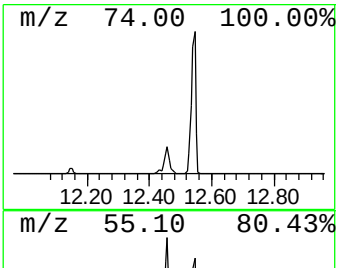
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 9-Octadecenoic acid (Z)-, m... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.46	55.47 ng	5597320	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99
3	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
4	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	99
5	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99





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Operator : JU/CG
Sample : L4007-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11929

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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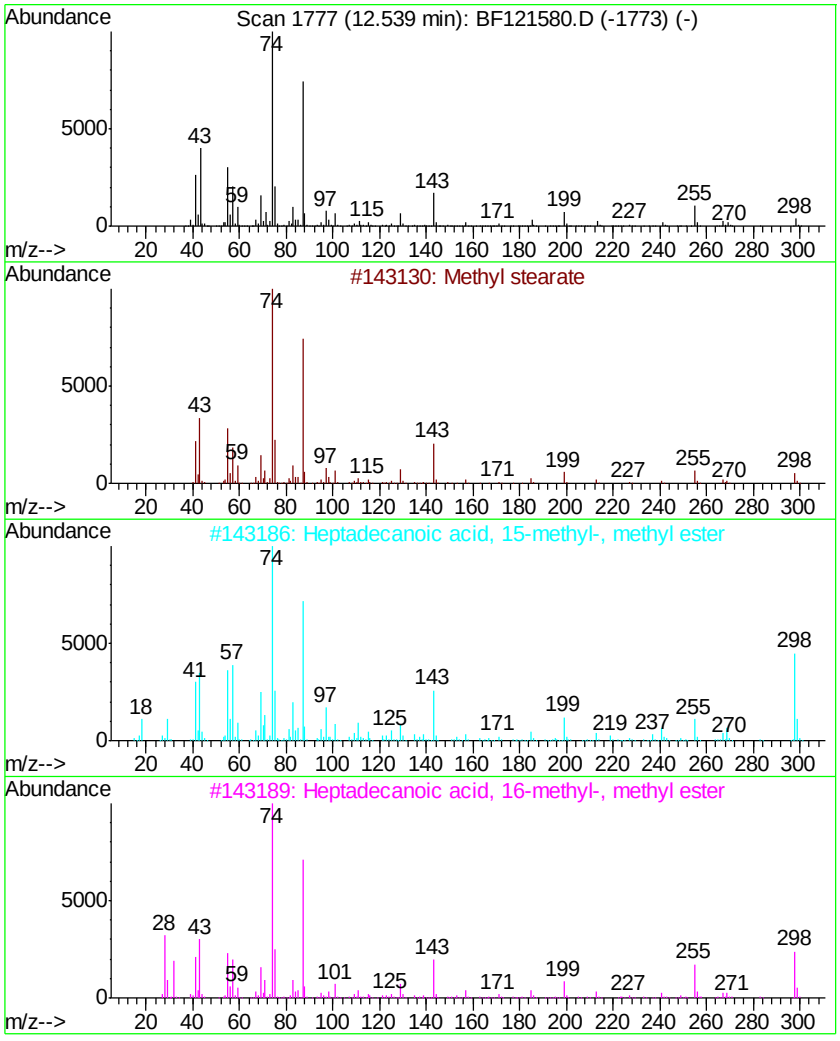
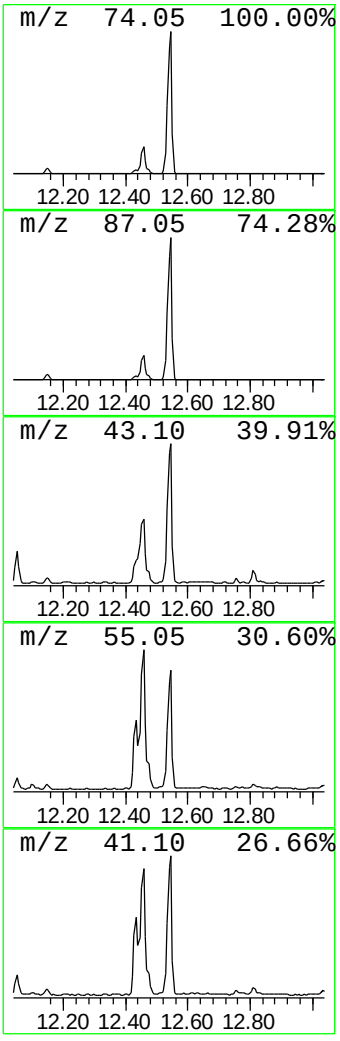
Peak Number 10 Methyl stearate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.54	69.54 ng	7017240	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	98
2	Heptadecanoic acid, 15-methyl-, ...	298	C19H38O2	054833-55-5	91
3	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	91
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	87
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	87





Library Search Compound Report

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Acq On : 15 Sep 2020 16:30
Operator : JU/CG
Sample : L4007-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11929

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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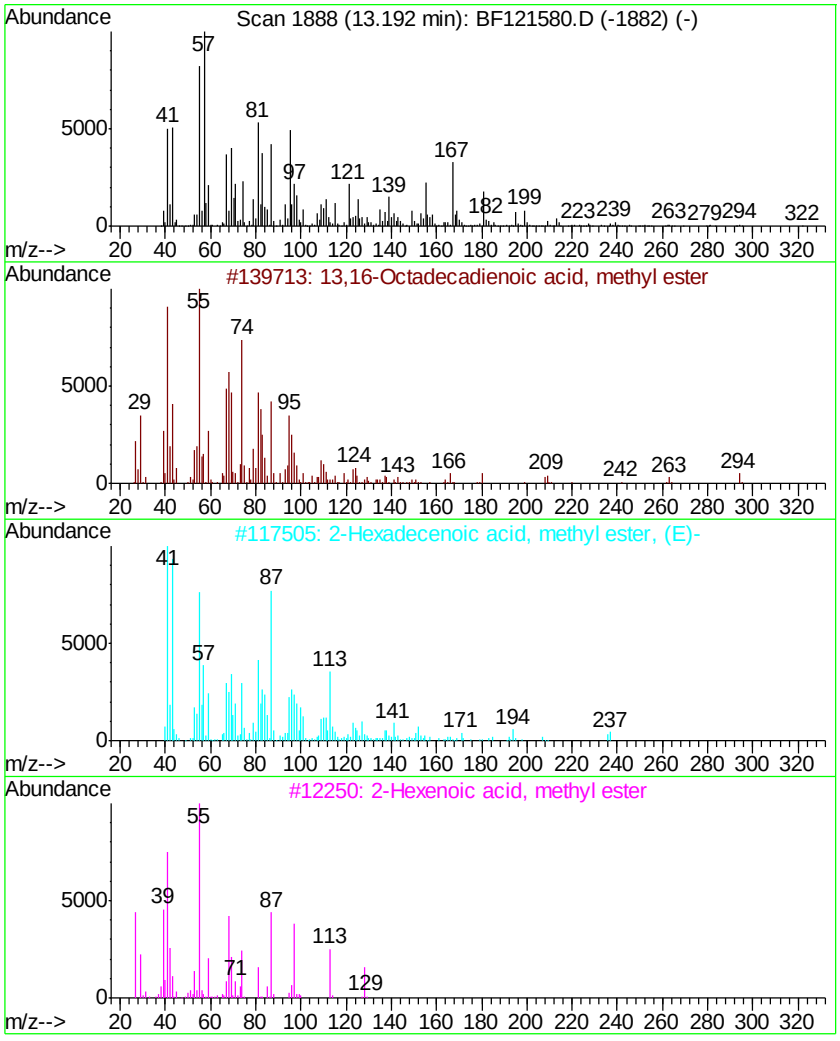
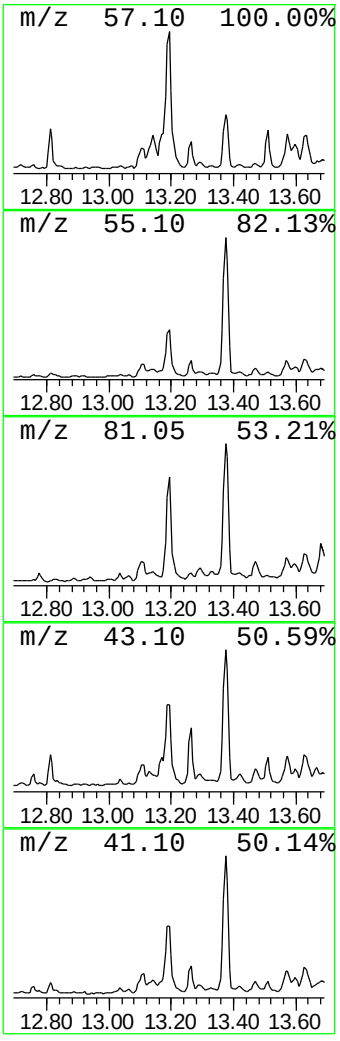
Peak Number 11 unknown13.19 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.19	47.97 ng	3767990	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13,16-Octadecadienoic acid, meth...	294	C19H34O2	056846-99-2	25
2	2-Hexadecenoic acid, methyl este...	268	C17H32O2	002825-81-2	22
3	2-Hexenoic acid, methyl ester	128	C7H12O2	002396-77-2	22
4	2-Heptenoic acid, methyl ester, ...	142	C8H14O2	038693-91-3	20
5	Oxiraneundecanoic acid, 3-pentyl...	312	C19H36O3	038520-30-8	16





Library Search Compound Report

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Acq On : 15 Sep 2020 16:30
Operator : JU/CG
Sample : L4007-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11929

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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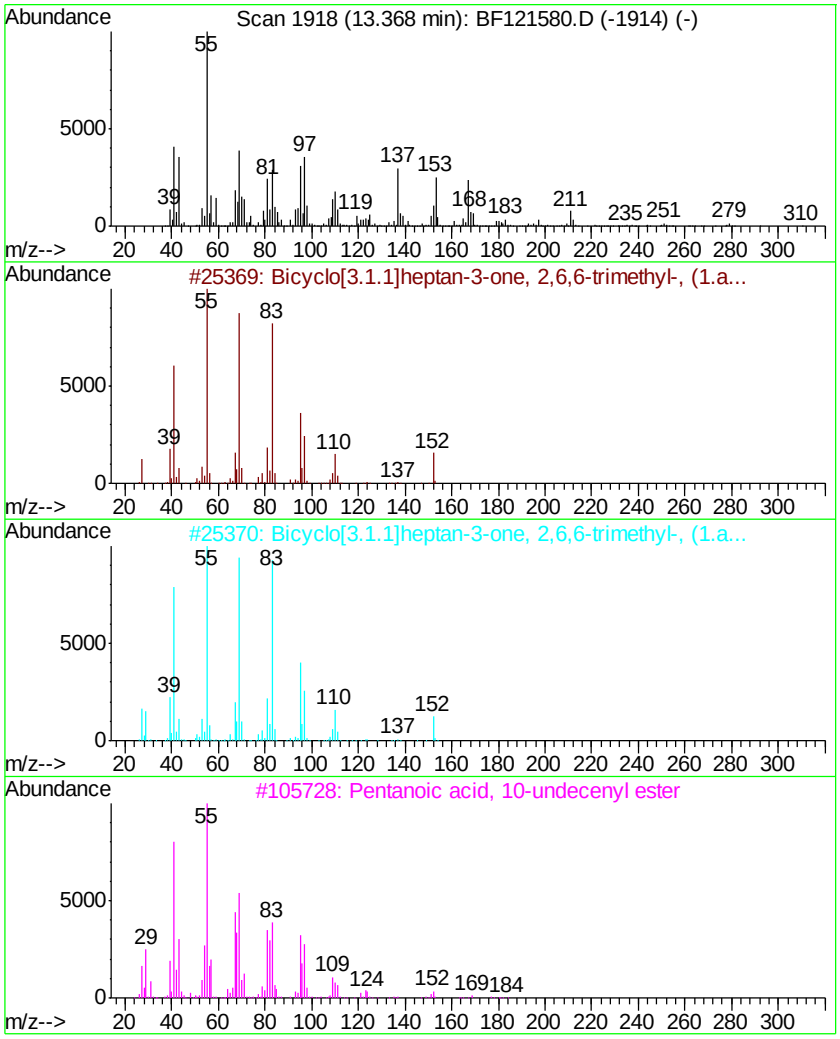
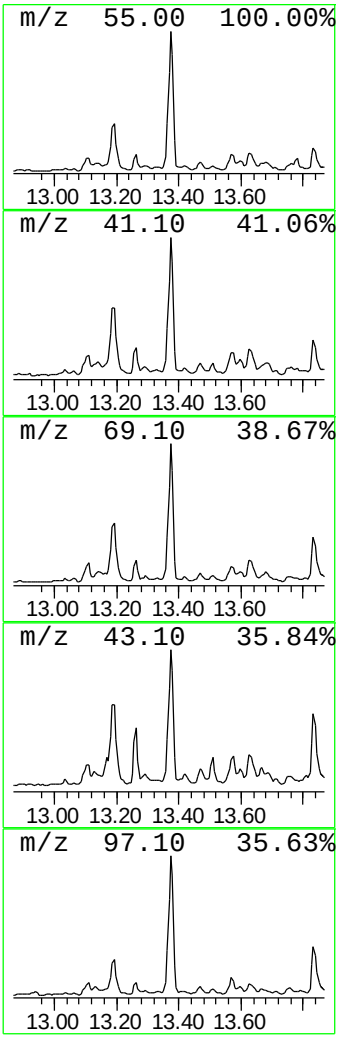
Peak Number 12 unknown13.37 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.37	70.97 ng	5574140	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	015358-88-0	35
2	Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	000547-60-4	27
3	Pentanoic acid, 10-undecenyl ester	254	C16H30O2	1000159-93-4	22
4	Cyclohexanemethanol, 4-methyl-, ...	128	C8H16O	003937-48-2	12
5	1,2-Ethanediamine, N-(5-nitro-2-...	182	C7H10N4O2	029602-39-9	11





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Sample : L4007-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11929

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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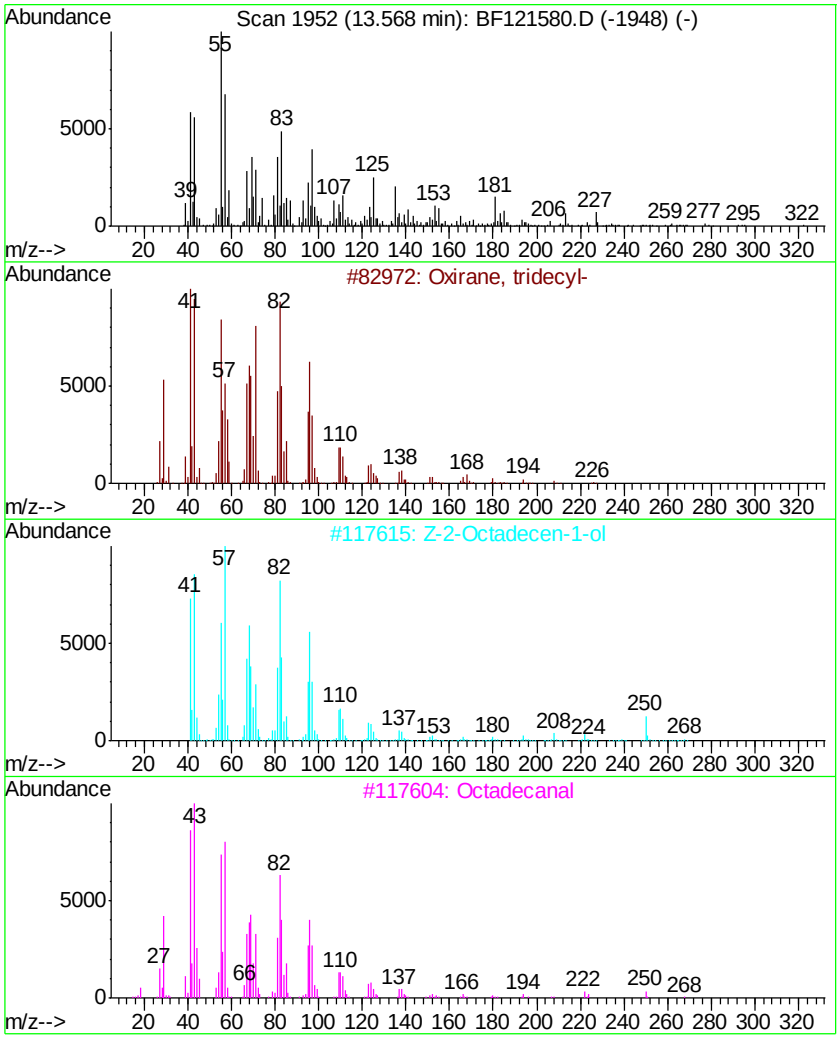
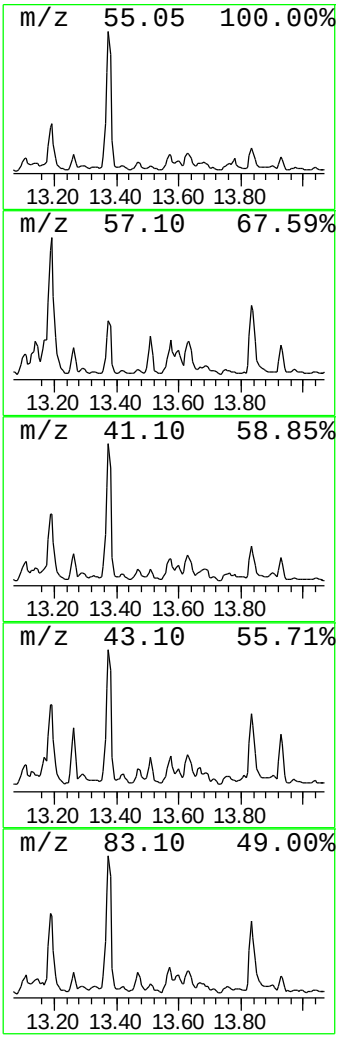
Peak Number 13 Oxirane, tridecyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.57	13.18 ng	1035540	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, tridecyl-	226	C15H30O	018633-25-5	78
2	Z-2-Octadecen-1-ol	268	C18H36O	1000131-11-0	45
3	Octadecanal	268	C18H36O	000638-66-4	43
4	2-Thiopheneacetic acid, 4-tridec...	324	C19H32O2S	1000280-66-8	38
5	2,3-Dimethyldodecane	198	C14H30	006117-98-2	38





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Operator : JU/CG
Sample : L4007-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11929

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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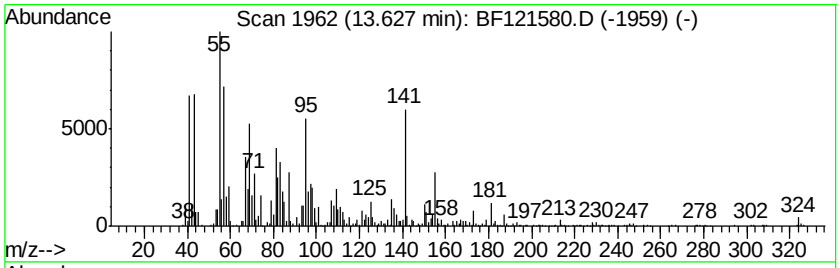
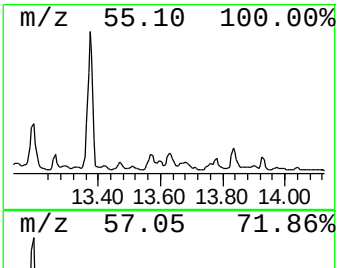
Peak Number 14 unknown13.63 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.63	13.14 ng	1031990	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-11-Hexadecenal	238	C16H30O	053939-28-9	35
2	Hydrazinecarboxamide, 2-cyclopen...	141	C6H11N3O	005459-00-7	30
3	Benzene, 1-fluoro-2-nitro-	141	C6H4FNO2	001493-27-2	27
4	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	25
5	2-Furoic acid, oct-3-en-2-yl ester	222	C13H18O3	1000299-23-6	25





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Sample : L4007-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11929

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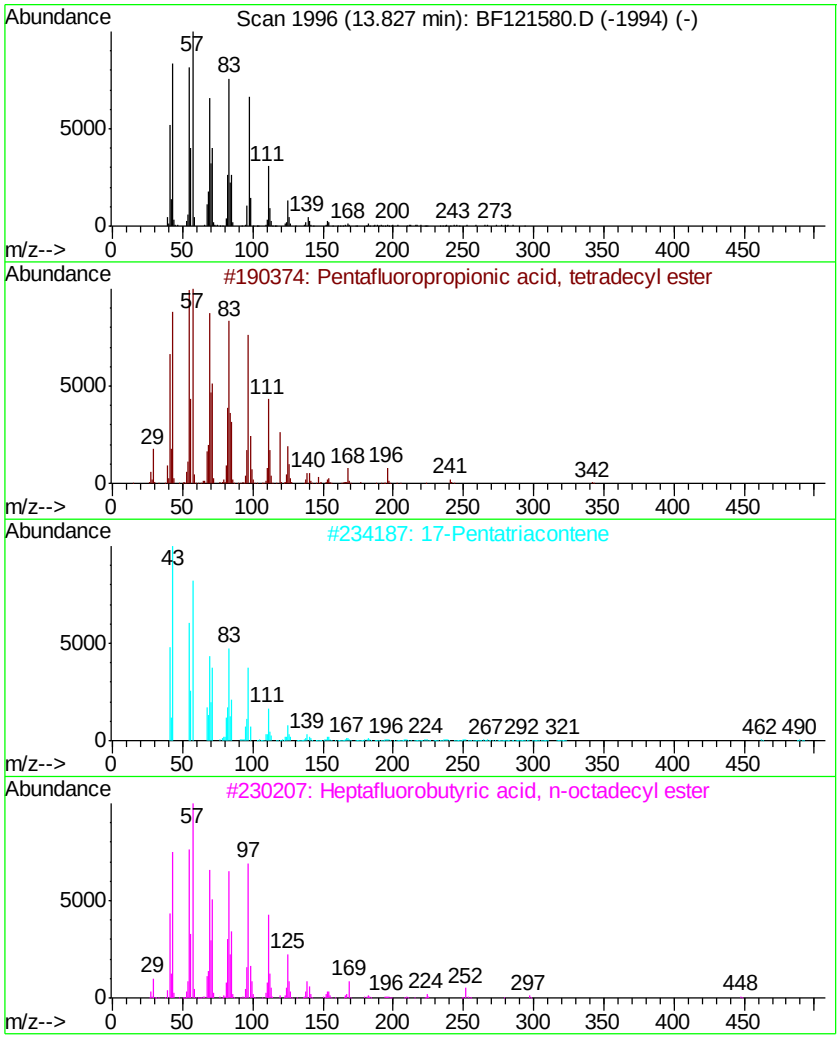
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

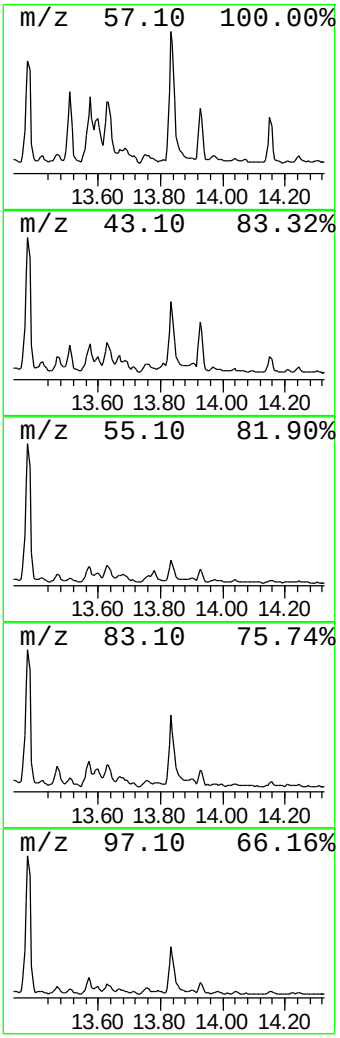
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 Pentafluoropropionic acid, ... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	15.53 ng	1219800	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	91
2	17-Pentatriacontene	491	C35H70	006971-40-0	91
3	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
4	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91





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ClientSampleId : 72-11929

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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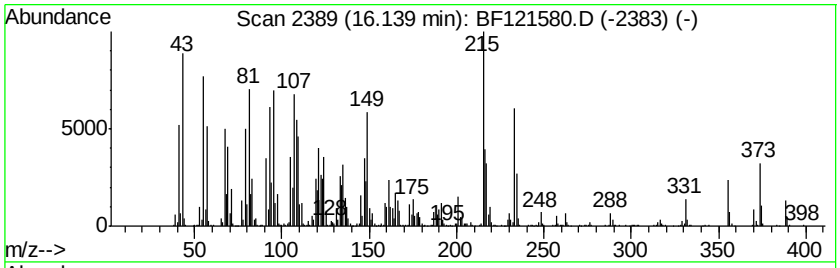
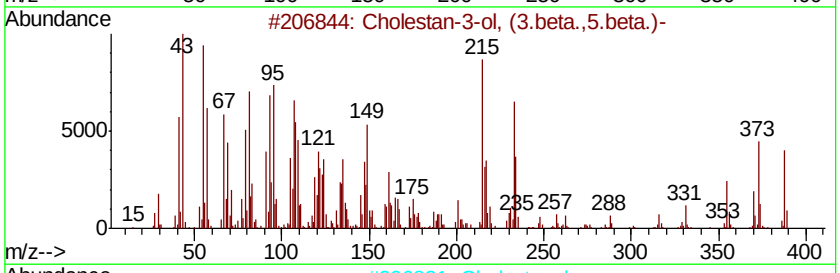
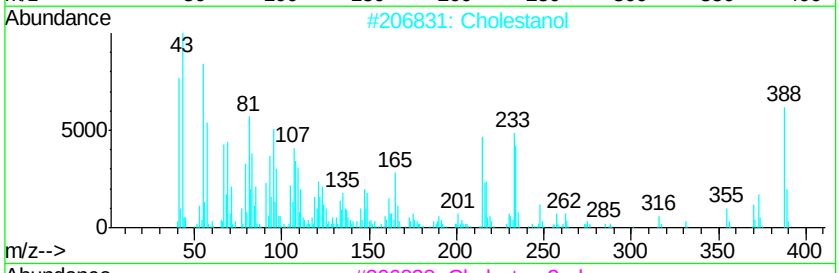
Peak Number 16 Cholestan-3-ol, (3.beta.,5.... Concentration Rank 2

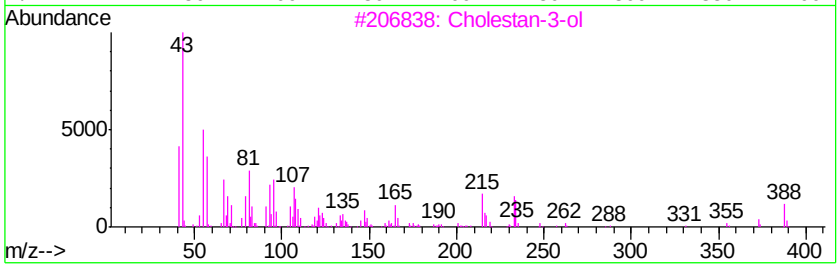
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.14	73.19 ng	4399580	Perylene-d12	15.44

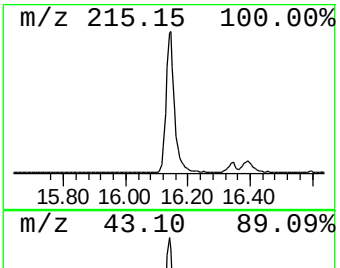
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholestan-3-ol, (3.beta.,5.beta.)-	388	C27H48O	000360-68-9	60
2	Cholestanol	388	C27H48O	000080-97-7	58
3	Cholestan-3-ol	388	C27H48O	027409-41-2	53
4	Cholestan-3-ol, (3.alpha.,5.beta.)-	388	C27H48O	000516-92-7	43
5	cis-3-[2-Hydroxy-4-(2-methyl-2-n...	332	C22H36O2	1000370-41-9	38

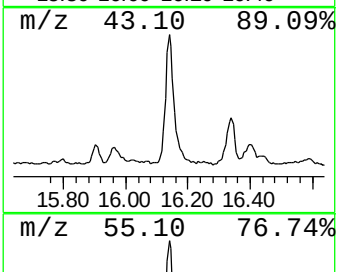


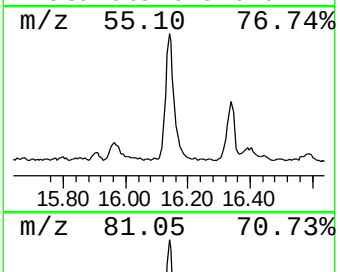


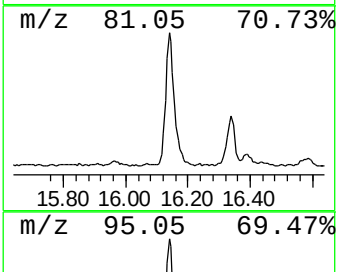


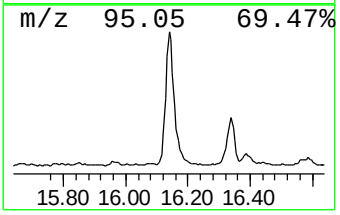












Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091520\
Data File : BF121580.D
Acq On : 15 Sep 2020 16:30
Operator : JU/CG
Sample : L4007-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11929

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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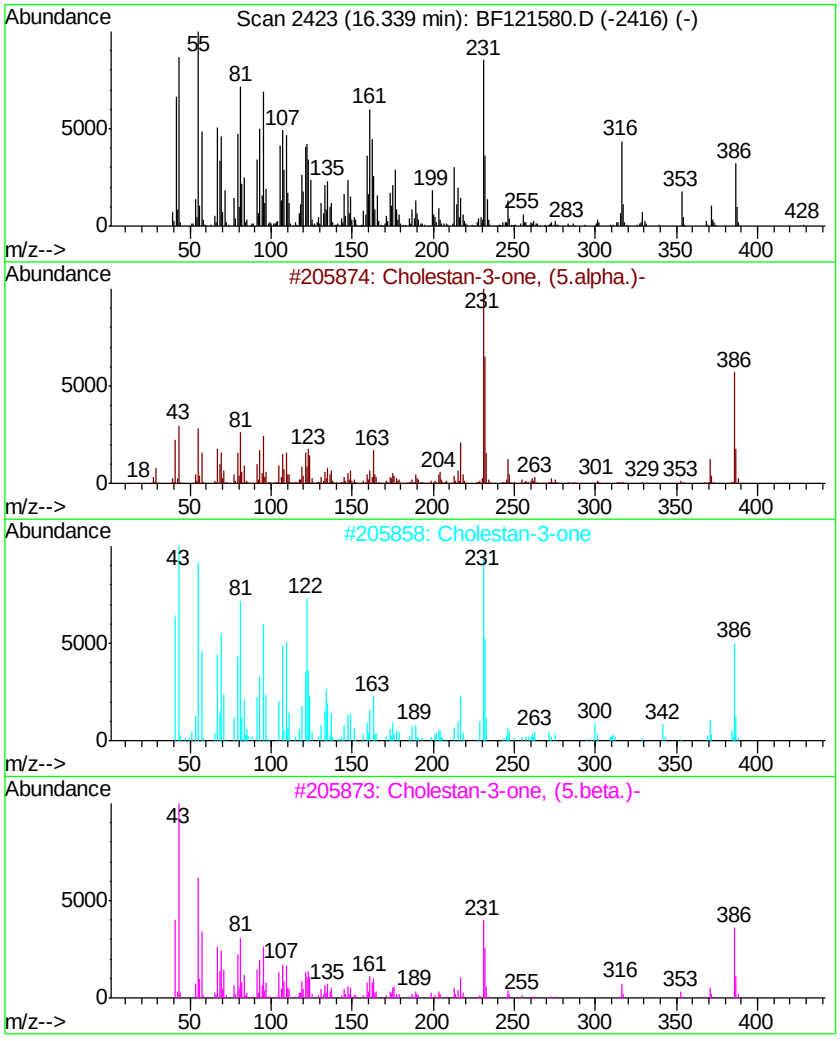
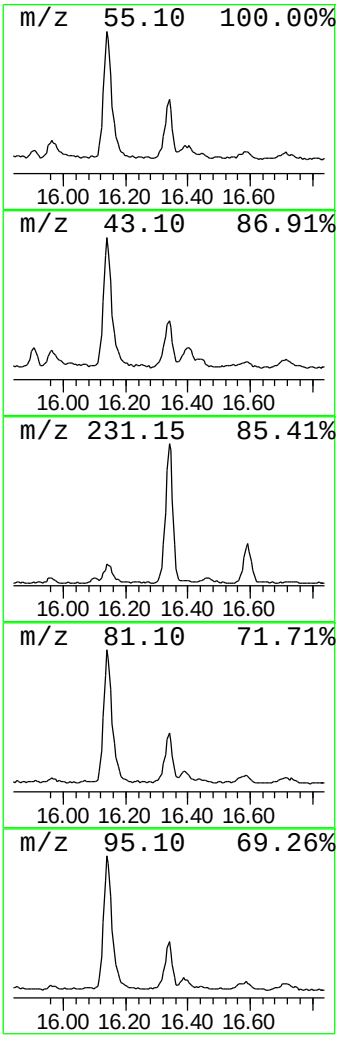
Peak Number 17 Cholestan-3-one, (5.alpha.)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.34	24.24 ng	1457010	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholestan-3-one, (5.alpha.)-	386	C27H46O	000566-88-1	86
2	Cholestan-3-one	386	C27H46O	015600-08-5	53
3	Cholestan-3-one, (5.beta.)-	386	C27H46O	000601-53-6	52
4	Cholestane, 4,5-epoxy-, (4.alpha...	386	C27H46O	006079-19-2	44
5	Cholestane-3,5-diol, (3.beta.,5....	404	C27H48O2	003347-60-2	38





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091520\
Data File : BF121580.D
Acq On : 15 Sep 2020 16:30
Operator : JU/CG
Sample : L4007-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11929

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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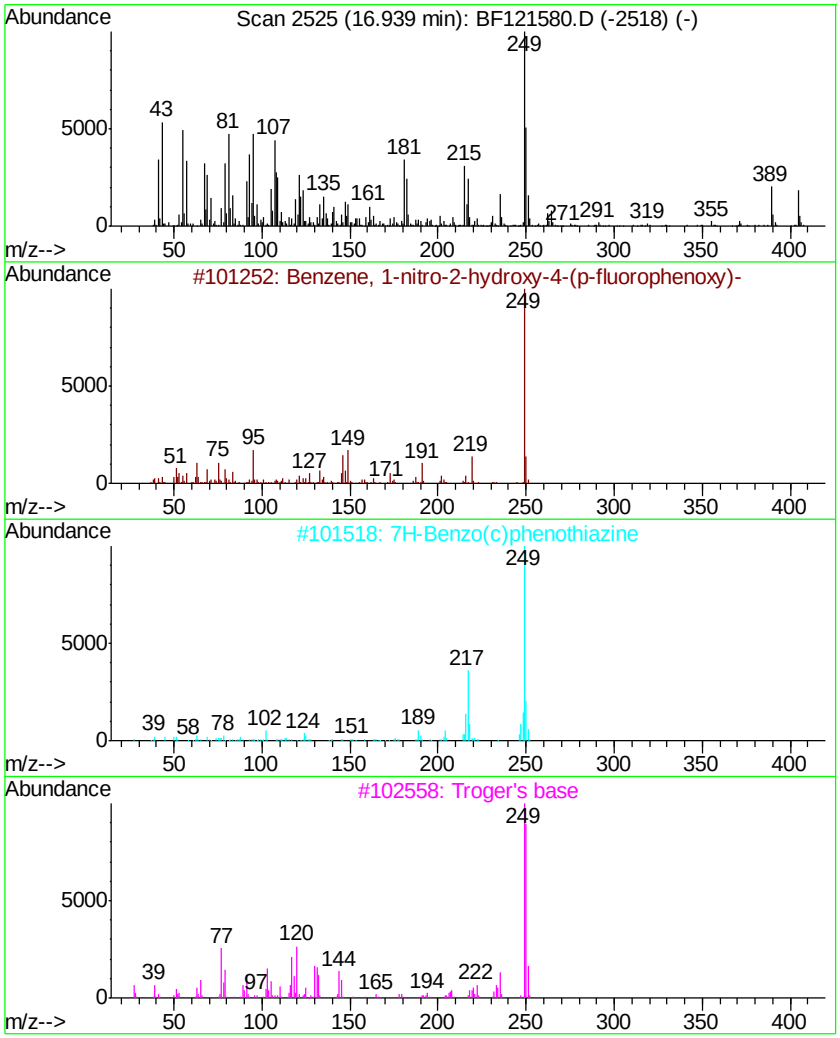
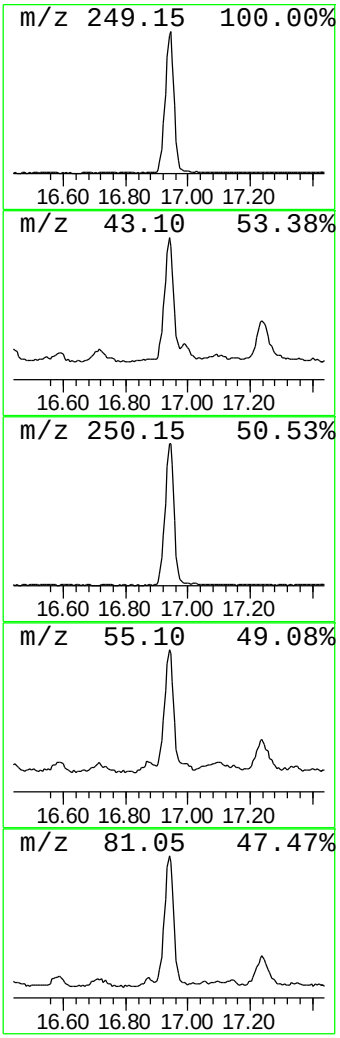
Peak Number 18 unknown16.94 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.94	54.81 ng	3294830	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-nitro-2-hydroxy-4-(p-...	249	C12H8FNO4	189214-56-0	35
2	7H-Benzo(c)phenothiazine	249	C16H11NS	000226-06-2	27
3	Troger's base	250	C17H18N2	072151-03-2	22
4	1H-Pyrazole-3-acetic acid, 1-(4-...	250	C12H11FN2O3	1000338-24-4	18
5	12H-Benzo(b)phenothiazine	249	C16H11NS	000258-08-2	16





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091520\
Data File : BF121580.D
Acq On : 15 Sep 2020 16:30
Operator : JU/CG
Sample : L4007-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11929

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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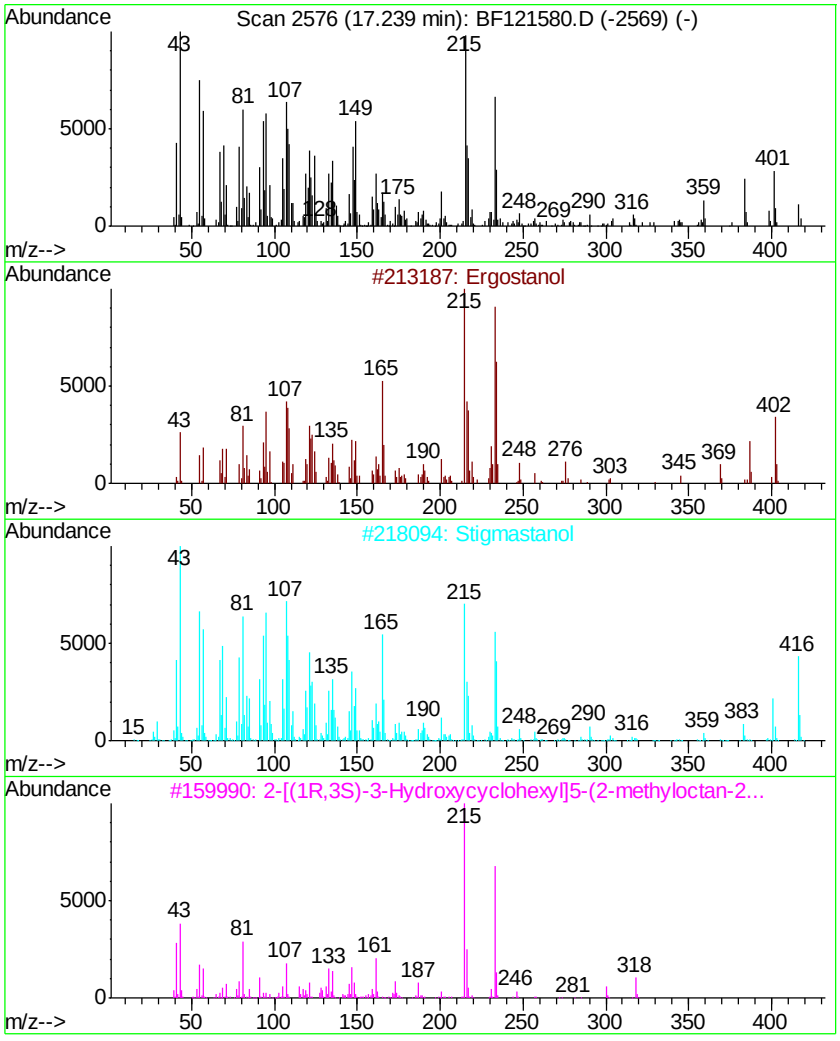
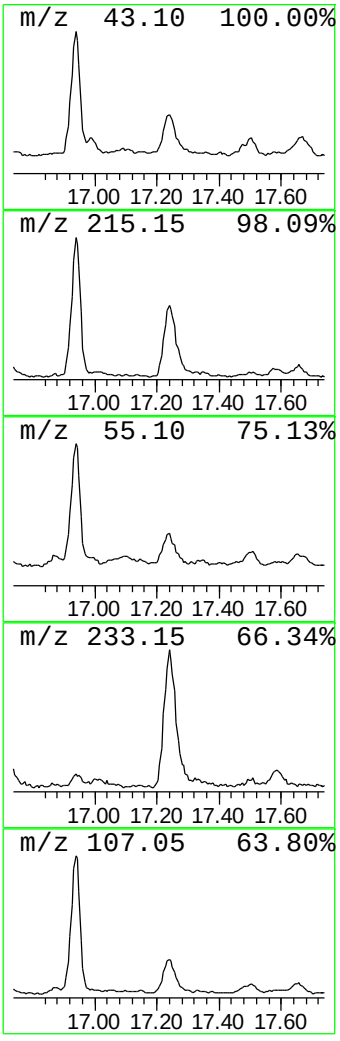
Peak Number 19 Ergostanol Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.24	17.55 ng	1054900	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ergostanol	402	C28H50O	006538-02-9	50
2	Stigmastanol	416	C29H52O	019466-47-8	47
3	2-[(1R,3S)-3-Hydroxycyclohexyl]5...	318	C21H34O2	070434-82-1	38
4	Cyclopent[e]-1,3-oxazine, octahy...	216	C13H16N2O	1000138-92-2	38
5	2-((1S,3R)-3-hydroxycyclohexyl)-...	332	C22H36O2	1000372-26-4	32





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091520\
Data File : BF121580.D
Acq On : 15 Sep 2020 16:30
Operator : JU/CG
Sample : L4007-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11929

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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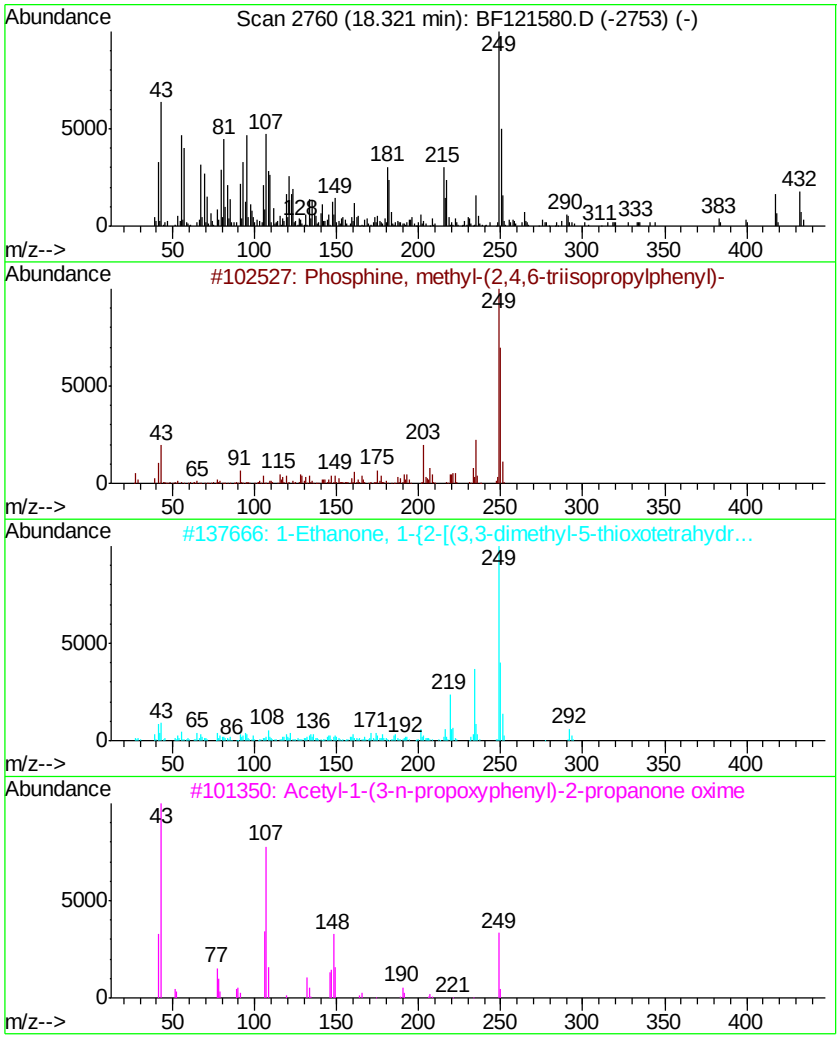
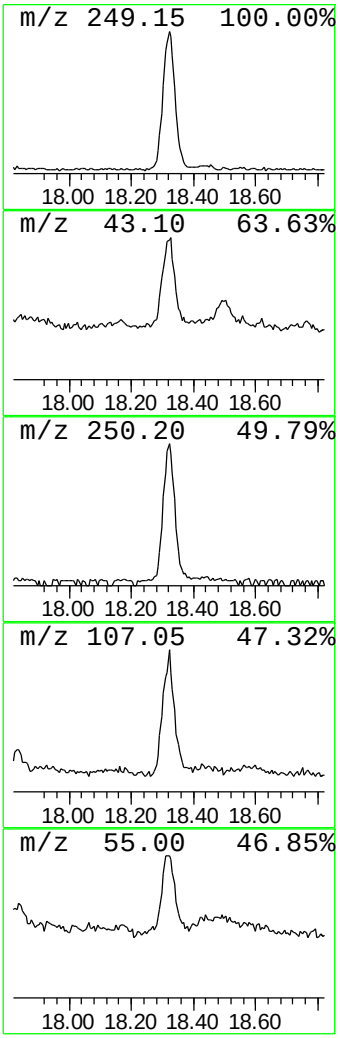
Peak Number 20 unknown18.32 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.32	12.27 ng	737487	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phosphine, methyl-(2,4,6-triisop...	250	C16H27P	158748-69-7	46
2	1-Ethanone, 1-{2-[(3,3-dimethyl-...	292	C16H24N2OS	077109-20-7	38
3	Acetyl-1-(3-n-propoxyphenyl)-2-p...	249	C14H19NO3	1000122-90-2	32
4	Benzene, 1-nitro-2-hydroxy-4-(p-...	249	C12H8FNO4	189214-56-0	32
5	2,4,6(1H,3H,5H)-Pyrimidinetrione...	264	C14H20N2O3	055044-42-3	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091520\
Data File : BF121580.D
Acq On : 15 Sep 2020 16:30
Operator : JU/CG
Sample : L4007-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11929

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.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
3-Penten-2-one, 4...	4.43	27.6	ng	1854440	1	6.83	1345710	20.0
2-Pentanone, 4-hy...	5.06	59.3	ng	3991610	1	6.83	1345710	20.0
Hexadecane	9.27	12.5	ng	1192120	3	9.87	1905200	20.0
Tetradecane	9.80	13.2	ng	1259510	3	9.87	1905200	20.0
Undecane, 2-methyl-	10.30	16.4	ng	1560440	3	9.87	1905200	20.0
Heptadecane	10.77	20.5	ng	2069140	4	11.35	2018100	20.0
Hexadecanoic acid...	11.76	92.4	ng	9320210	4	11.35	2018100	20.0
9,12-Octadecadien...	12.43	41.8	ng	4221970	4	11.35	2018100	20.0
9-Octadecenoic ac...	12.46	55.5	ng	5597320	4	11.35	2018100	20.0
Methyl stearate	12.54	69.5	ng	7017240	4	11.35	2018100	20.0
unknown13.19	13.19	48.0	ng	3767990	5	13.99	1570910	20.0
unknown13.37	13.37	71.0	ng	5574140	5	13.99	1570910	20.0
Oxirane, tridecyl-	13.57	13.2	ng	1035540	5	13.99	1570910	20.0
unknown13.63	13.63	13.1	ng	1031990	5	13.99	1570910	20.0
Pentafluoropropio...	13.83	15.5	ng	1219800	5	13.99	1570910	20.0
Cholestan-3-ol, (...	16.14	73.2	ng	4399580	6	15.44	1202320	20.0
Cholestan-3-one, ...	16.34	24.2	ng	1457010	6	15.44	1202320	20.0
unknown16.94	16.94	54.8	ng	3294830	6	15.44	1202320	20.0
Ergostanol	17.24	17.6	ng	1054900	6	15.44	1202320	20.0
unknown18.32	18.32	12.3	ng	737487	6	15.44	1202320	20.0