LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061820\
Data File : BF120646.D
Acq On : 18 Jun 2020 17:11
Operator : JU/CG
Sample : L3034-14
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5

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-BF061020.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	5.410	560	565	569	rBV	3189051	3425659	83.04%	10.850%
2	6.434	734	739	742	rBV	3223563	3442680	83.46%	10.904%
3	6.798	797	801	805	rBV	1153442	893541	21.66%	2.830%
4	6.957	824	828	831	rBV	3568263	3015037	73.09%	9.550%
5	7.363	892	897	900	rBV	2601859	2308004	55.95%	7.310%
6	8.081	1015	1019	1022	rBV	1412614	1103901	26.76%	3.496%
7	9.157	1197	1202	1205	rBV	4663128	4125143	100.00%	13.066%
8	9.545	1265	1268	1272	rBV	239076	240238	5.82%	0.761%
9	9.833	1313	1317	1322	rVB	1306934	1000230	24.25%	3.168%
10	10.622	1447	1451	1457	rBV	2290081	2197418	53.27%	6.960%
11	10.751	1468	1473	1475	rVB	58636	64392	1.56%	0.204%
12	11.063	1522	1526	1530	rBV6	23069	44814	1.09%	0.142%
13	11.216	1550	1552	1559	rVB	86489	75985	1.84%	0.241%
14	11.316	1566	1569	1573	rBV	1100590	1030298	24.98%	3.263%
15	11.669	1627	1629	1634	rVB5	61803	58478	1.42%	0.185%
16	11.933	1670	1674	1677	rBV4	63243	88176	2.14%	0.279%
17	12.016	1686	1688	1693	rBV5	59528	82675	2.00%	0.262%
18	12.239	1724	1726	1728	rBV2	67505	71081	1.72%	0.225%
19	12.292	1733	1735	1737	rBV2	68630	54560	1.32%	0.173%
20	12.363	1745	1747	1750	rBV2	84801	75171	1.82%	0.238%
21	12.398	1750	1753	1754	rBV3	52578	55434	1.34%	0.176%
22	12.457	1761	1763	1767	rBV4	52316	64626	1.57%	0.205%
23	12.721	1805	1808	1812	rBV5	115340	198359	4.81%	0.628%
24	12.757	1812	1814	1818	rVV2	109346	153665	3.73%	0.487%
25	12.810	1821	1823	1826	rVV3	59311	69585	1.69%	0.220%
26	12.904	1835	1839	1842	rVV	3725483	3565359	86.43%	11.293%
27	12.933	1842	1844	1848	rVB4	94373	95453	2.31%	0.302%
28	13.074	1866	1868	1872	rBV4	123332	193254	4.68%	0.612%
29	13.139	1878	1879	1882	rBV3	102772	72150	1.75%	0.229%
30	13.210	1889	1891	1892	rBV2	125668	117757	2.85%	0.373%
31	13.433	1928	1929	1933	rBV3	100358	113851	2.76%	0.361%
32	13.557	1949	1950	1952	rBV2	105828	84311	2.04%	0.267%
33	13.957	2014	2018	2021	rBV	1002255	1057724	25.64%	3.350%
34	14.215	2059	2062	2066	rBV3	186670	213667	5.18%	0.677%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061820\
Data File : BF120646.D
Acq On : 18 Jun 2020 17:11
Operator : JU/CG
Sample : L3034-14
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5

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-BF061020.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.404	2093	2094	2097	rBV3	225945	228300	5.53%	0.723%
36	14.592	2123	2126	2127	rBV3	256010	349737	8.48%	1.108%
37	14.763	2151	2155	2158	rBV2	213618	284887	6.91%	0.902%
38	14.792	2158	2160	2165	rVB4	212795	208630	5.06%	0.661%
39	15.039	2199	2202	2204	rBV3	268033	341939	8.29%	1.083%
40	15.404	2260	2264	2273	rVB	504018	706532	17.13%	2.238%

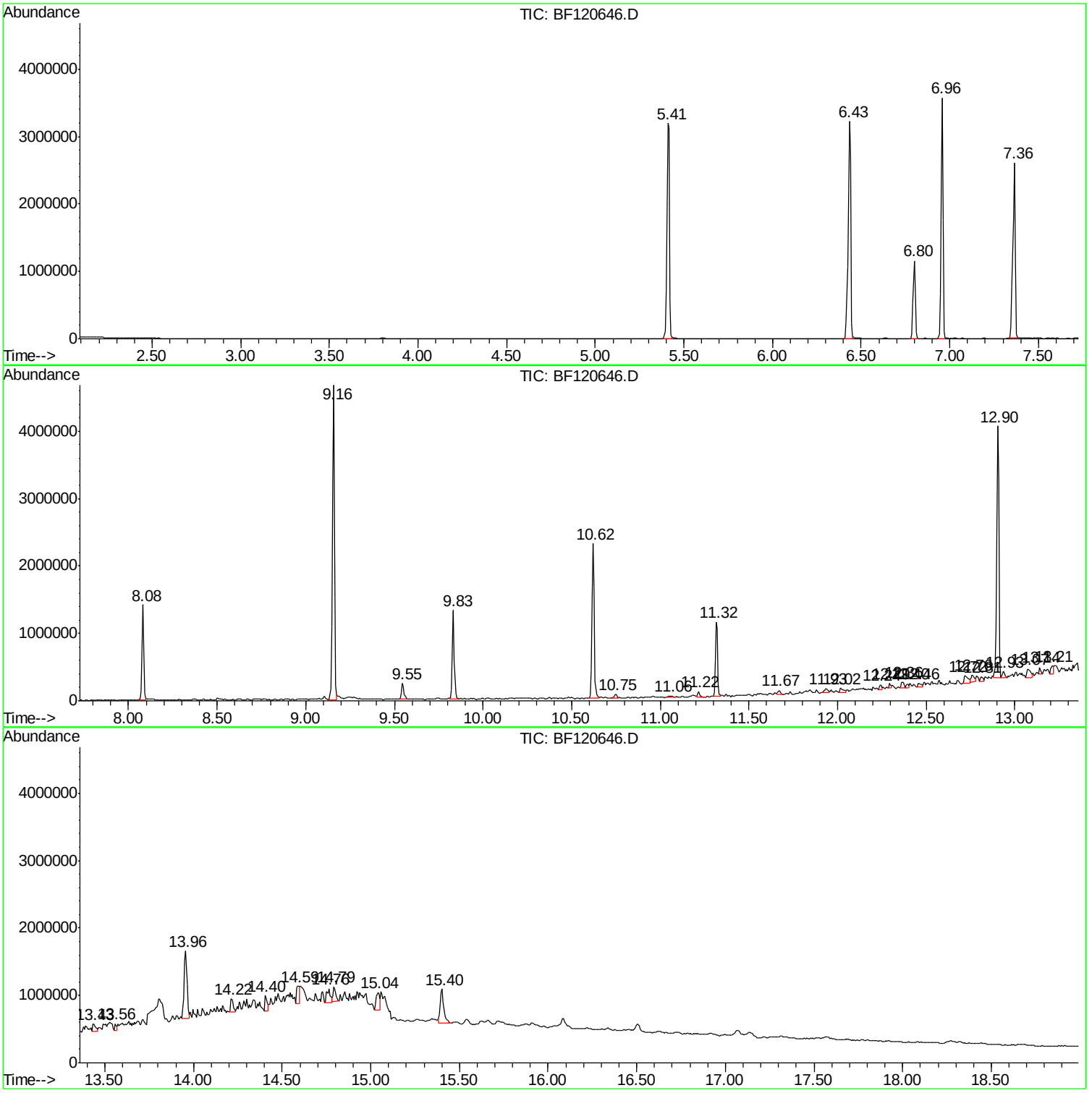
Sum of corrected areas: 31572701

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061820\
Data File : BF120646.D
Acq On : 18 Jun 2020 17:11
Operator : JU/CG
Sample : L3034-14
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061820\
Data File : BF120646.D
Acq On : 18 Jun 2020 17:11
Operator : JU/CG
Sample : L3034-14
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

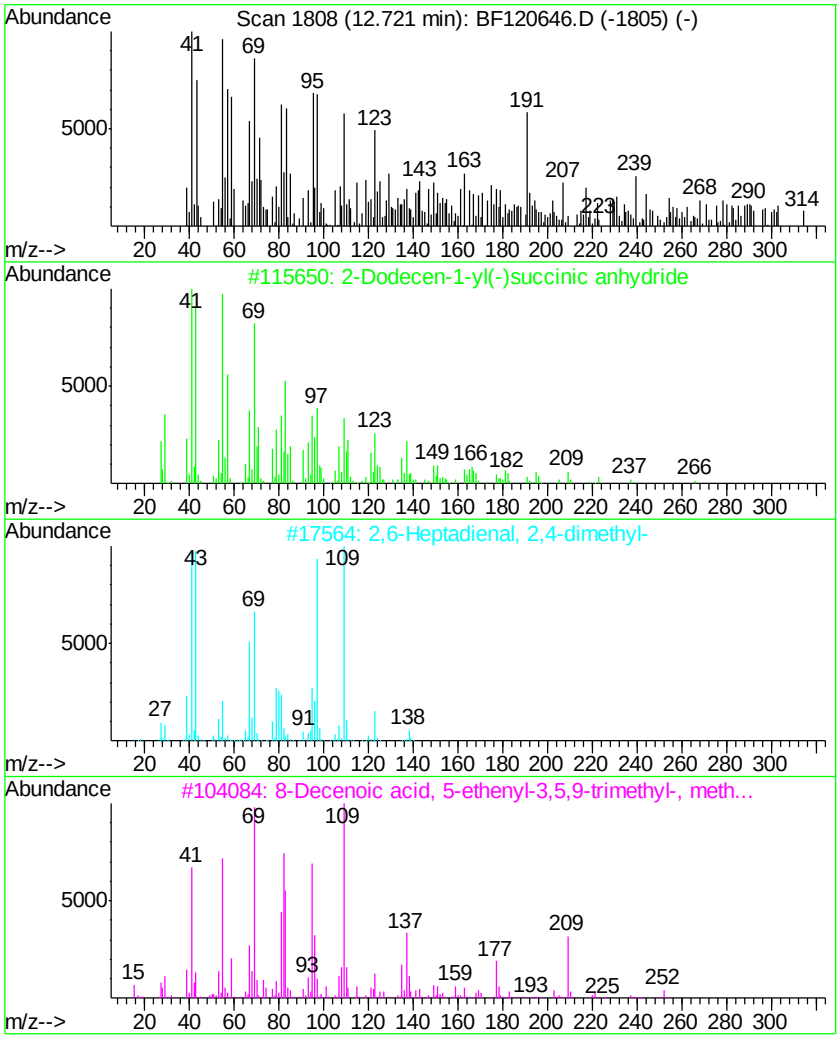
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

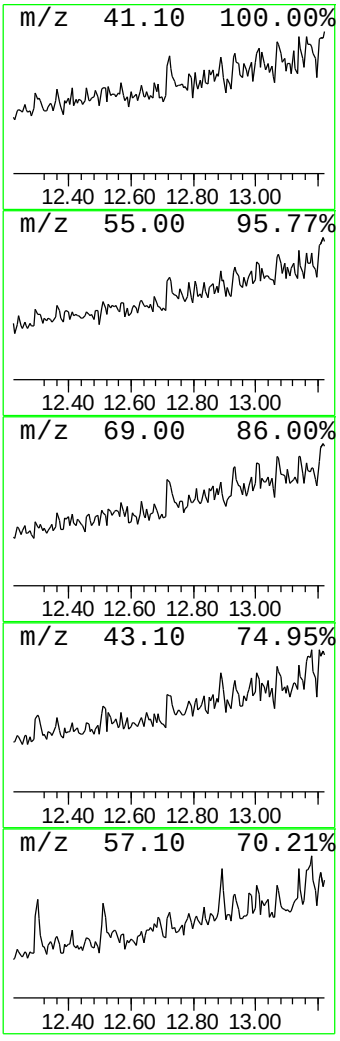
****

Peak Number 2 unknown12.72 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.72	3.75 ng	198359	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Dodecen-1-yl(-)succinic anhydride	266	C16H26O3	019780-11-1	46
2	2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	45
3	8-Decenoic acid, 5-ethenyl-3,5,9...	252	C16H28O2	056114-53-5	45
4	Methyl Camphorsulfonates	246	C11H18O4S	046471-67-4	41
5	3-Cyclohexene-1-carboxaldehyde, ...	152	C10H16O	040702-26-9	40





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061820\
Data File : BF120646.D
Acq On : 18 Jun 2020 17:11
Operator : JU/CG
Sample : L3034-14
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

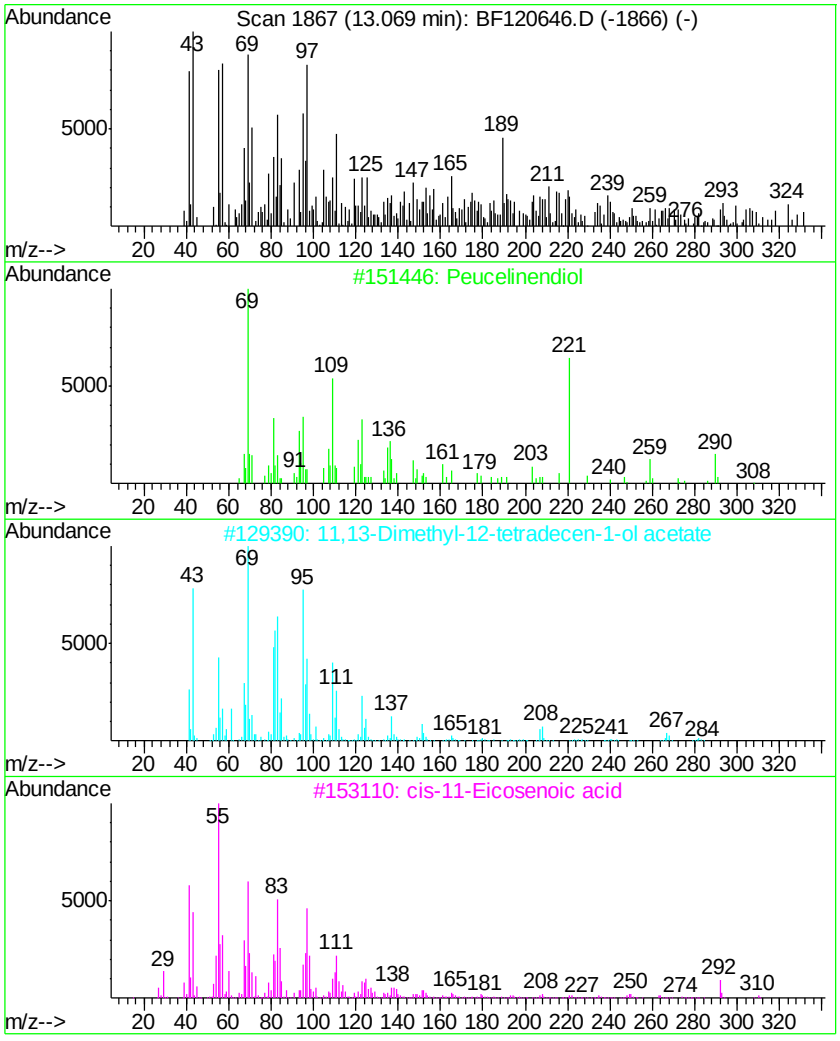
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

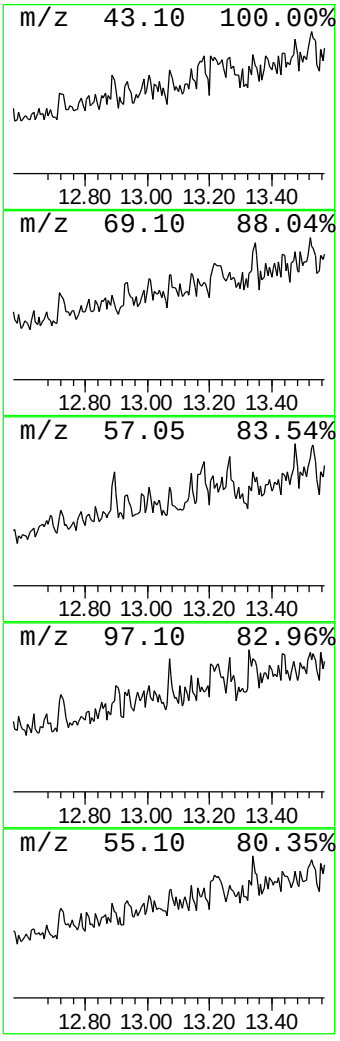
****

Peak Number 4 Peucelinendiol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.07	3.65 ng	193254	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Peucelinendiol	308	C20H36O2	072776-48-8	53
2	11,13-Dimethyl-12-tetradecen-1-o...	282	C18H34O2	1000130-81-0	38
3	cis-11-Eicosenoic acid	310	C20H38O2	005561-99-9	25
4	Cyclohexanebutanoic acid, 2,2-di...	224	C14H24O2	095452-15-6	25
5	cis-13-Eicosenoic acid	310	C20H38O2	017735-94-3	25





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061820\
Data File : BF120646.D
Acq On : 18 Jun 2020 17:11
Operator : JU/CG
Sample : L3034-14
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

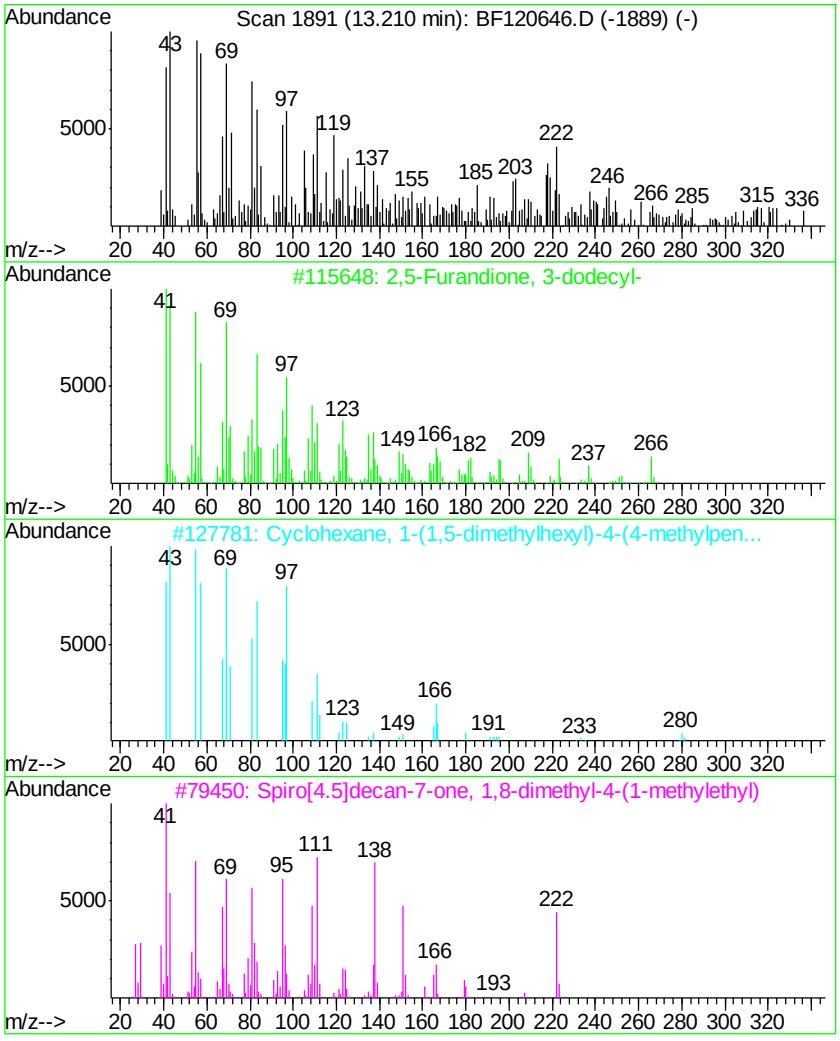
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

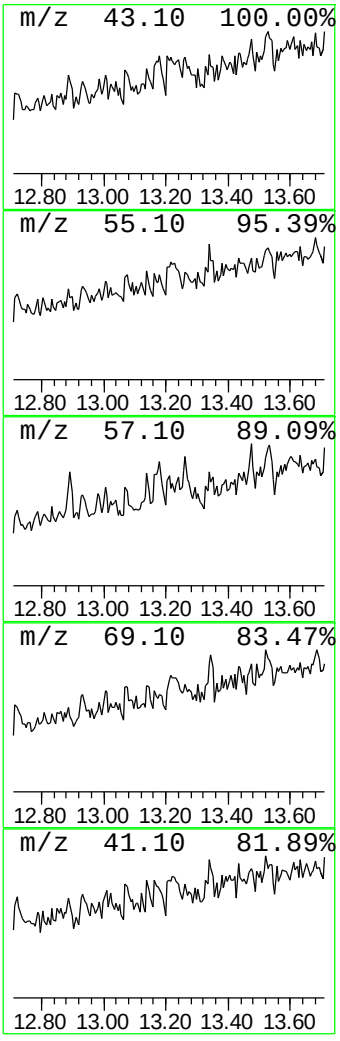
****

Peak Number 5 2,5-Furandione, 3-dodecyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.21	2.23 ng	117757	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Furandione, 3-dodecyl-	266	C16H26O3	059426-46-9	53
2	Cyclohexane, 1-(1,5-dimethylhexy...	280	C20H40	056009-20-2	38
3	Spiro[4.5]decan-7-one, 1,8-dimet...	222	C15H26O	039510-26-4	35
4	Hexadecanoic acid, 2-hydroxy-, m...	286	C17H34O3	016742-51-1	35
5	n-Propyl 11-octadecenoate	324	C21H40O2	1000336-71-7	30





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061820\
Data File : BF120646.D
Acq On : 18 Jun 2020 17:11
Operator : JU/CG
Sample : L3034-14
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

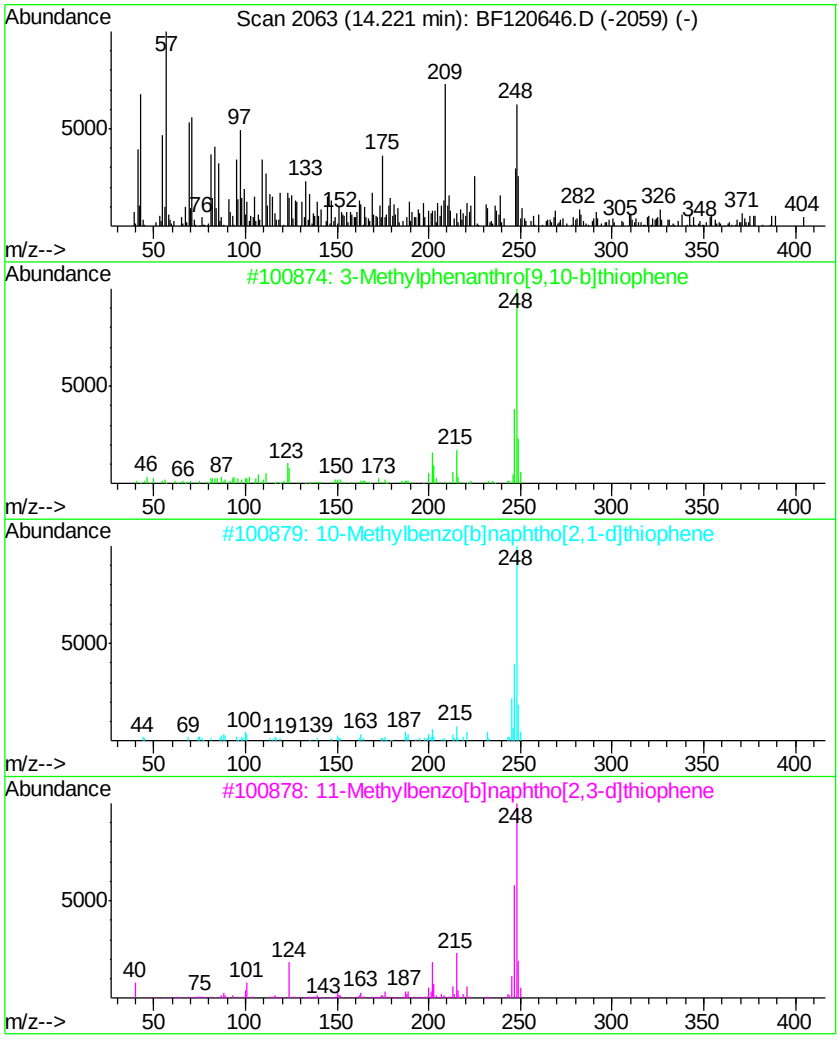
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

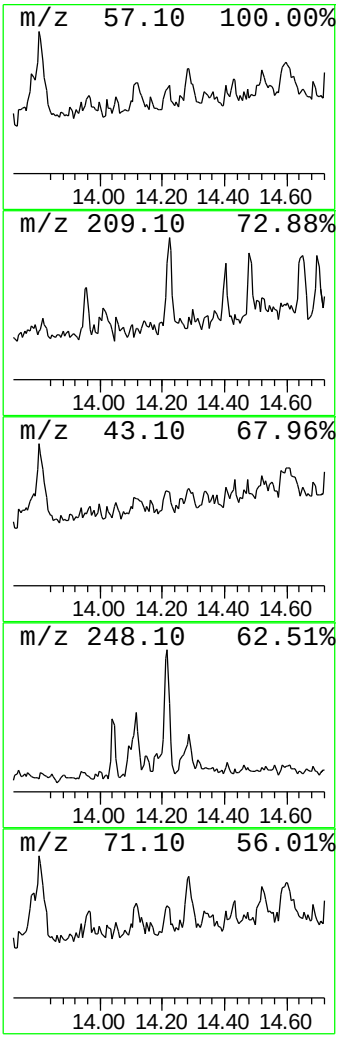
****

Peak Number 7 3-Methylphenanthro[9,10-b]t... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.22	4.04 ng	213667	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Methylphenanthro[9,10-b]thiophene	248	C17H12S	082420-70-0	95
2	10-Methylbenzo[b]naphtho[2,1-d]t...	248	C17H12S	083821-58-3	78
3	11-Methylbenzo[b]naphtho[2,3-d]t...	248	C17H12S	079966-33-9	70
4	7-Methyl-5-oxo-2-phenyl-3,5-dihy...	248	C16H12N2O	1000301-27-7	62
5	3-Methylbenzo[b]naphtho[2,1-d]th...	248	C17H12S	004567-45-7	60





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061820\
Data File : BF120646.D
Acq On : 18 Jun 2020 17:11
Operator : JU/CG
Sample : L3034-14
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

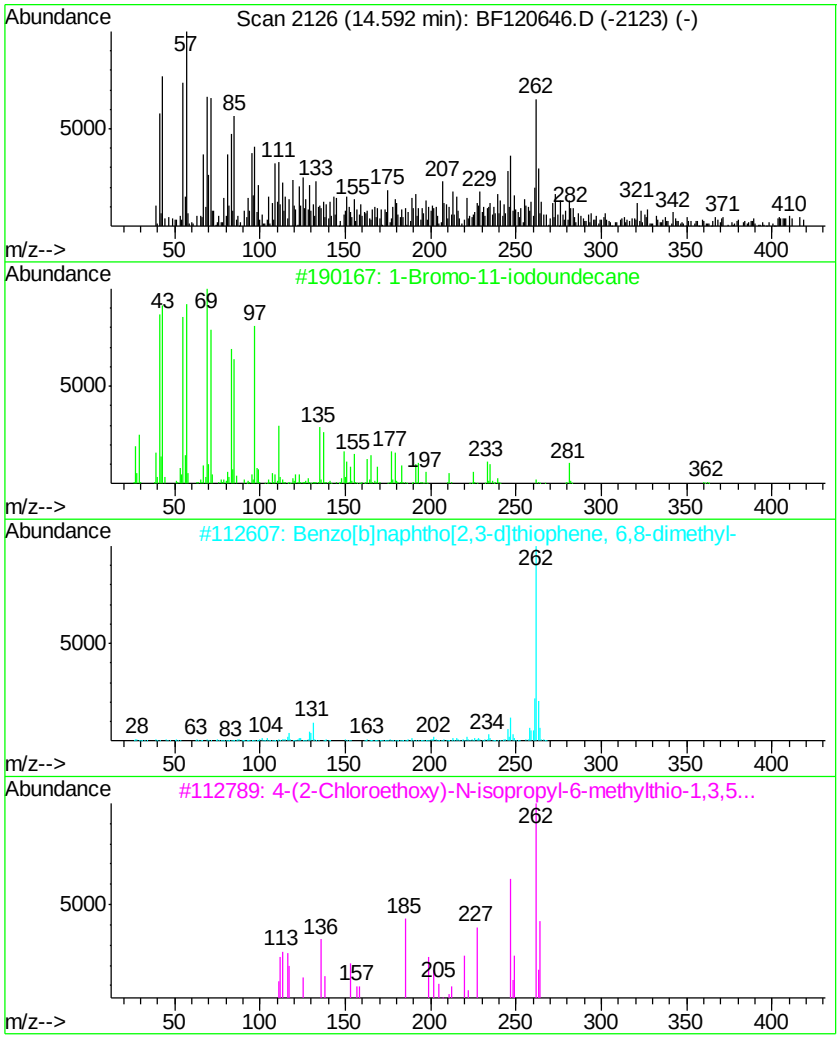
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

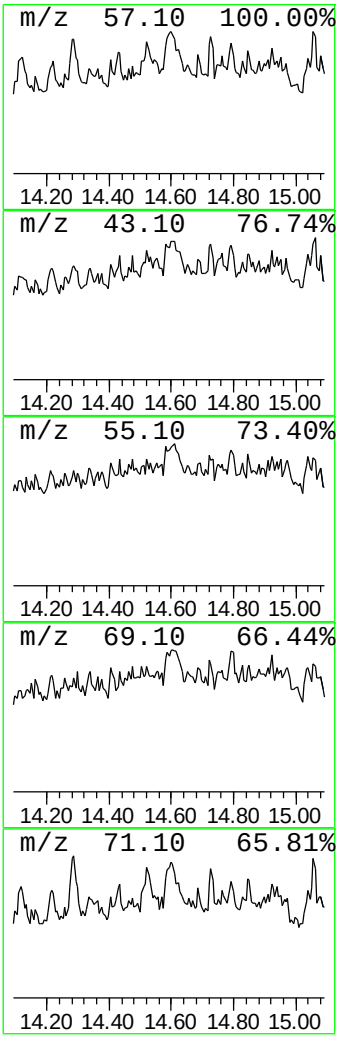
****

Peak Number 9 unknown14.59 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	6.61 ng	349737	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Bromo-11-iodoundecane	360	C11H22BrI	139123-69-6	46
2	Benzo[b]naphtho[2,3-d]thiophene,...	262	C18H14S	024964-16-7	41
3	4-(2-Chloroethoxy)-N-isopropyl-6...	262	C9H15ClN4OS	073775-70-9	41
4	2-Methyl-4-phenyl-6-(2-hydroxyph...	262	C17H14N2O	017432-80-3	35
5	Titanyl acetylacetonate	262	C10H14O5Ti	014024-64-7	30





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061820\
Data File : BF120646.D
Acq On : 18 Jun 2020 17:11
Operator : JU/CG
Sample : L3034-14
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

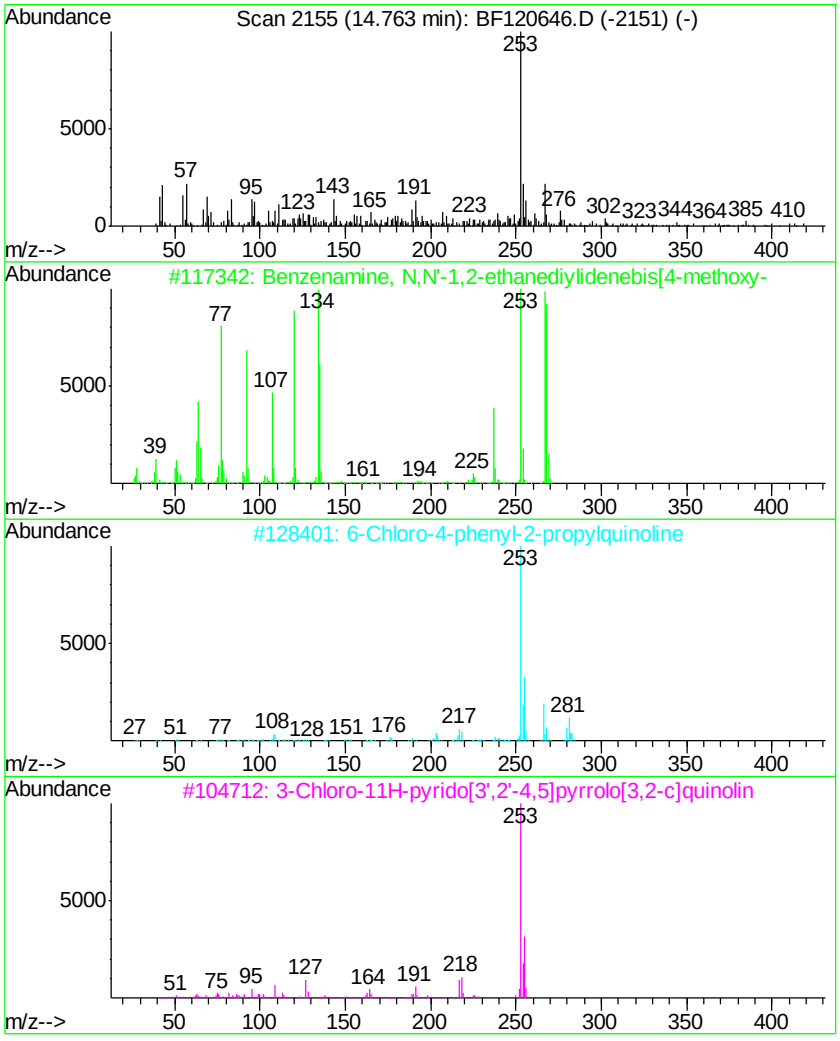
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

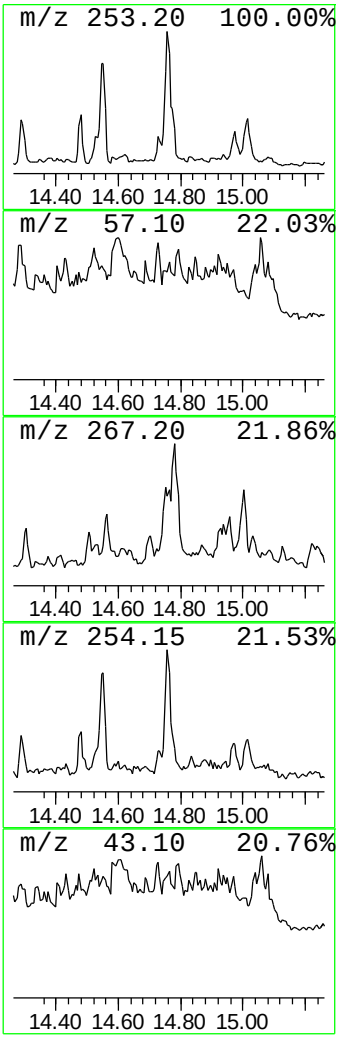
****

Peak Number 10 Benzenamine, N,N'-1,2-ethan... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.76	8.06 ng	284887	Perylene-d12	15.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenamine, N,N'-1,2-ethanediyl...	268	C16H16N2O2	024764-91-8	64
2	6-Chloro-4-phenyl-2-propylquinoline	281	C18H16ClN	022609-08-1	53
3	3-Chloro-11H-pyrido[3',2'-4,5]py...	253	C14H8ClN3	1000212-59-4	52
4	Succinic acid, 2-methylphenyl 2-...	360	C23H20O4	1000357-54-3	52
5	Benz(a)anthracene-7-carbonitrile	253	C19H11N	007476-08-6	50





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061820\
Data File : BF120646.D
Acq On : 18 Jun 2020 17:11
Operator : JU/CG
Sample : L3034-14
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

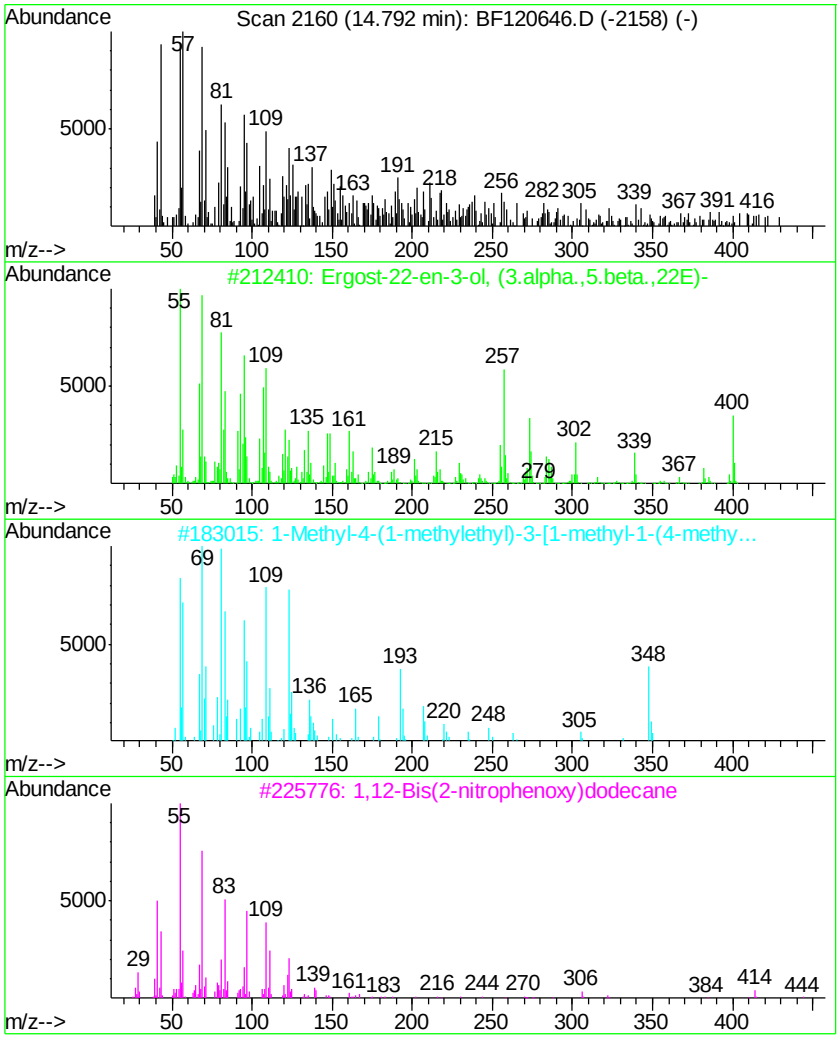
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

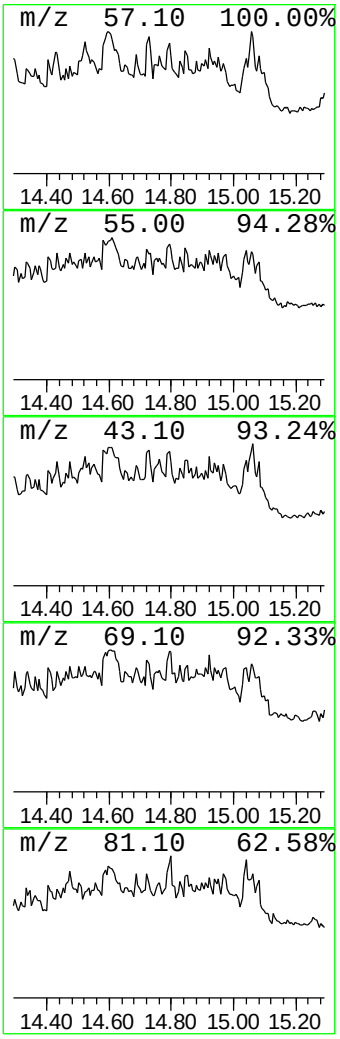
****

Peak Number 11 Ergost-22-en-3-ol, (3.alpha... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	5.91 ng	208630	Perylene-d12	15.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ergost-22-en-3-ol, (3.alpha.,5.b...	400	C28H48O	055527-92-9	83
2	1-Methyl-4-(1-methylethyl)-3-[1-...	348	C25H48	1000370-41-4	76
3	1,12-Bis(2-nitrophenoxy)dodecane	444	C24H32N2O6	155056-69-2	70
4	4-n-Hexylthiane, S,S-dioxide	218	C11H22O2S	070928-52-8	50
5	Cholestan-3-one, 4,4-dimethyl-, ...	414	C29H50O	002097-85-0	49





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061820\
Data File : BF120646.D
Acq On : 18 Jun 2020 17:11
Operator : JU/CG
Sample : L3034-14
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

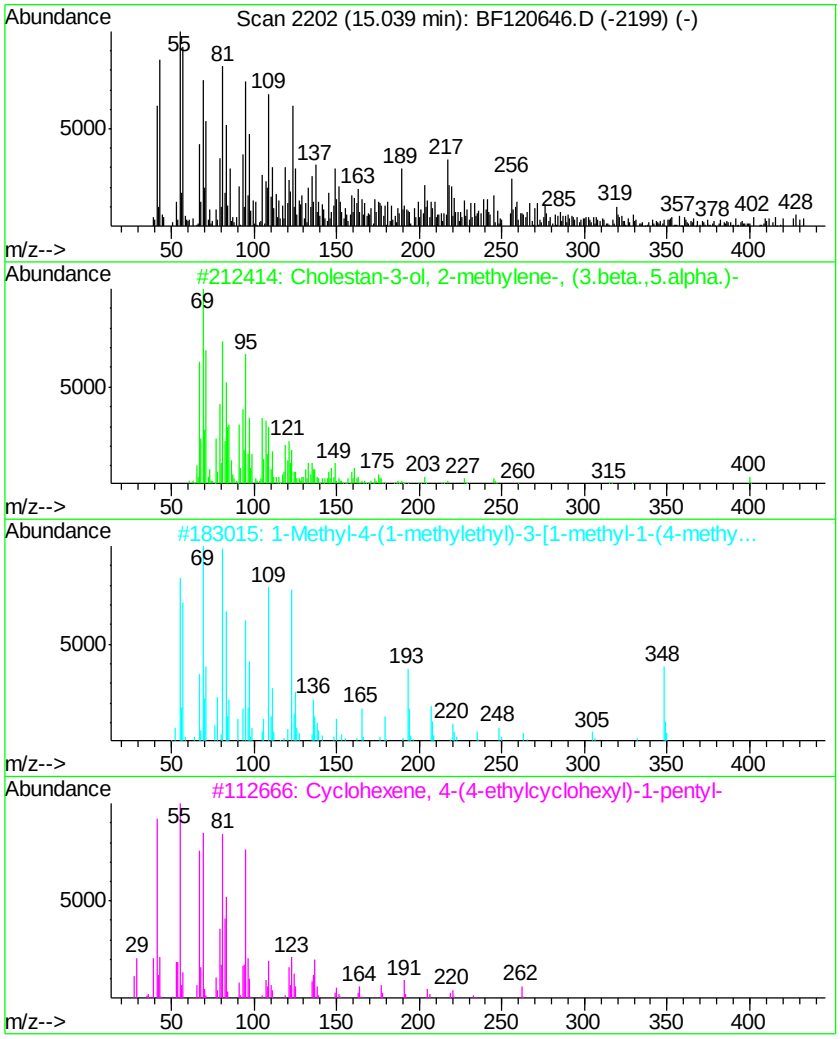
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

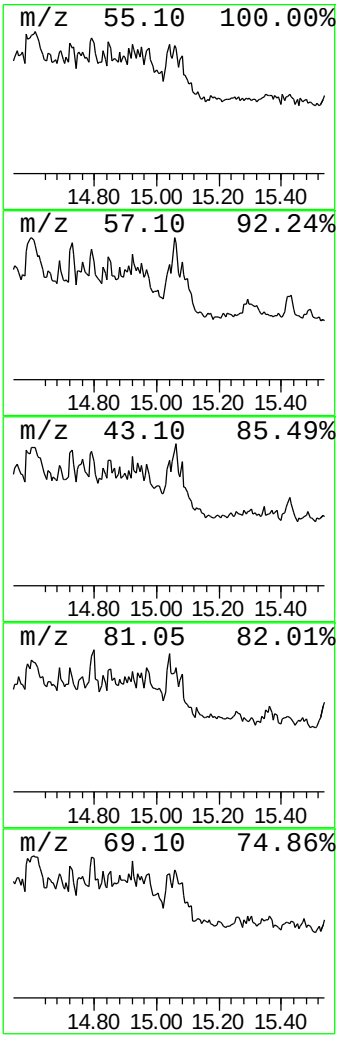
****

Peak Number 12 Cholestan-3-ol, 2-methylene... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.04	9.68 ng	341939	Perylene-d12	15.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholestan-3-ol, 2-methylene-, (3...	400	C28H48O	022599-96-8	87
2	1-Methyl-4-(1-methylethyl)-3-[1-...	348	C25H48	1000370-41-4	87
3	Cyclohexene, 4-(4-ethylcyclohexy...	262	C19H34	301643-32-3	70
4	1H-Indene, 5-butyl-6-hexyloctahy...	264	C19H36	055044-36-5	70
5	(2Z,4E)-3,7,11-Trimethyl-2,4,10-...	206	C15H26	172549-29-0	60





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF061820\
Data File : BF120646.D
Acq On : 18 Jun 2020 17:11
Operator : JU/CG
Sample : L3034-14
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061020.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
unknown12.72	12.72	3.8	ng	198359	5	13.96	1057720	20.0
Peucelinendiol	13.07	3.6	ng	193254	5	13.96	1057720	20.0
2,5-Furandione, 3...	13.21	2.2	ng	117757	5	13.96	1057720	20.0
3-Methylphenanthr...	14.22	4.0	ng	213667	5	13.96	1057720	20.0
unknown14.59	14.59	6.6	ng	349737	5	13.96	1057720	20.0
Benzenamine, N,N'...	14.76	8.1	ng	284887	6	15.40	706532	20.0
Ergost-22-en-3-ol...	14.79	5.9	ng	208630	6	15.40	706532	20.0
Cholestan-3-ol, 2...	15.04	9.7	ng	341939	6	15.40	706532	20.0