LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022020\
Data File : BF118987.D
Acq On : 21 Feb 2020 4:48
Operator : CG/JU
Sample : L1547-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MARCY-GREEN-BH-01-A

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-BF022020.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	4.975	487	491	499	rVB	28631	39377	1.15%	0.121%
2	5.387	557	561	574	rBV	2976703	2854944	83.66%	8.802%
3	6.404	730	734	751	rBV	2793277	2842552	83.29%	8.764%
4	6.763	791	795	804	rBV	1106786	928666	27.21%	2.863%
5	6.922	818	822	825	rBV	2800259	2499879	73.25%	7.707%
6	7.322	886	890	894	rBV	1854571	1822728	53.41%	5.619%
7	8.045	1009	1013	1016	rBV	1245124	1128495	33.07%	3.479%
8	9.116	1191	1195	1199	rBV	3661744	3412633	100.00%	10.521%
9	9.510	1259	1262	1266	rVB	135382	102739	3.01%	0.317%
10	9.657	1284	1287	1290	rBV	38539	37173	1.09%	0.115%
11	9.710	1290	1296	1299	rBV	25201	42775	1.25%	0.132%
12	9.798	1307	1311	1314	rBV	1326718	1226130	35.93%	3.780%
13	9.828	1314	1316	1319	rVB	46264	37644	1.10%	0.116%
14	10.580	1440	1444	1448	rBV	2141256	1894127	55.50%	5.840%
15	11.051	1520	1524	1527	rVB	110550	97183	2.85%	0.300%
16	11.139	1534	1539	1543	rBV6	24418	49758	1.46%	0.153%
17	11.274	1558	1562	1565	rBV	1096992	1115080	32.68%	3.438%
18	11.298	1565	1566	1571	rVV	397696	340519	9.98%	1.050%
19	11.351	1572	1575	1579	rVB	103995	101530	2.98%	0.313%
20	11.504	1597	1601	1607	rBV2	45783	66566	1.95%	0.205%
21	11.733	1638	1640	1644	rBV4	30022	39006	1.14%	0.120%
22	11.780	1645	1648	1650	rBV	58770	56957	1.67%	0.176%
23	11.810	1650	1653	1657	rBV	404345	393141	11.52%	1.212%
24	11.892	1663	1667	1669	rBV2	90466	93839	2.75%	0.289%
25	12.069	1693	1697	1700	rBV2	43884	70799	2.07%	0.218%
26	12.098	1700	1702	1707	rVV	40356	44953	1.32%	0.139%
27	12.327	1738	1741	1744	rBV2	53010	57806	1.69%	0.178%
28	12.416	1753	1756	1760	rBV	46610	51145	1.50%	0.158%
29	12.486	1765	1768	1771	rBV	806680	781366	22.90%	2.409%
30	12.592	1782	1786	1791	rBV3	122833	172387	5.05%	0.531%
31	12.716	1801	1807	1811	rBV	787689	809591	23.72%	2.496%
32	12.857	1827	1831	1835	rBV	2807835	2726498	79.89%	8.406%
33	13.045	1861	1863	1866	rVB2	96636	87737	2.57%	0.270%
34	13.110	1872	1874	1877	rBV	62701	46918	1.37%	0.145%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022020\
Data File : BF118987.D
Acq On : 21 Feb 2020 4:48
Operator : CG/JU
Sample : L1547-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MARCY-GREEN-BH-01-A

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-BF022020.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.716	1975	1977	1981	rBV2	198635	209182	6.13%	0.645%
36	13.763	1981	1985	1989	rVV2	301147	386746	11.33%	1.192%
37	13.915	2005	2011	2013	rBV2	1218099	1564507	45.84%	4.823%
38	13.939	2013	2015	2018	rVB	405047	313231	9.18%	0.966%
39	14.045	2030	2033	2036	rBV	290792	278391	8.16%	0.858%
40	14.080	2036	2039	2042	rVV	406717	436699	12.80%	1.346%
41	14.110	2042	2044	2046	rVV2	157005	145012	4.25%	0.447%
42	14.133	2046	2048	2053	rVB3	175474	205655	6.03%	0.634%
43	14.751	2151	2153	2158	rVB	361883	343586	10.07%	1.059%
44	14.939	2182	2185	2192	rVB	399718	662412	19.41%	2.042%
45	15.004	2193	2196	2199	rBV	516906	565783	16.58%	1.744%
46	15.351	2251	2255	2267	rVB	693238	1252273	36.70%	3.861%

Sum of corrected areas: 32436118

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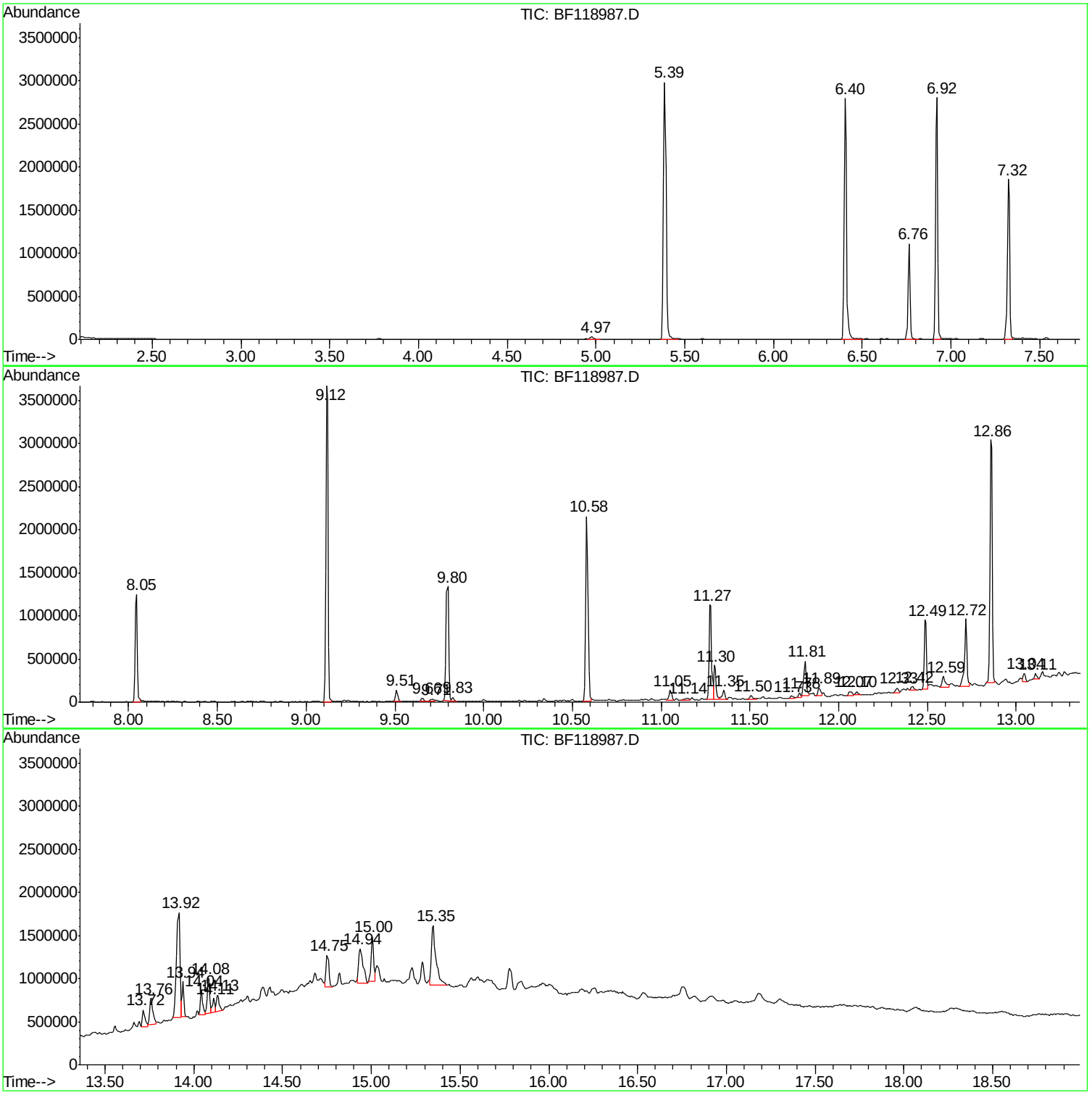
Instrument :
BNA_F
ClientSampleId :
MARCY-GREEN-BH-01-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.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\BF022020\
Data File : BF118987.D
Acq On : 21 Feb 2020 4:48
Operator : CG/JU
Sample : L1547-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MARCY-GREEN-BH-01-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

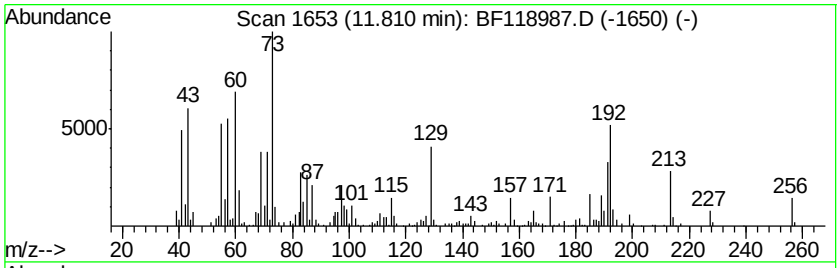
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

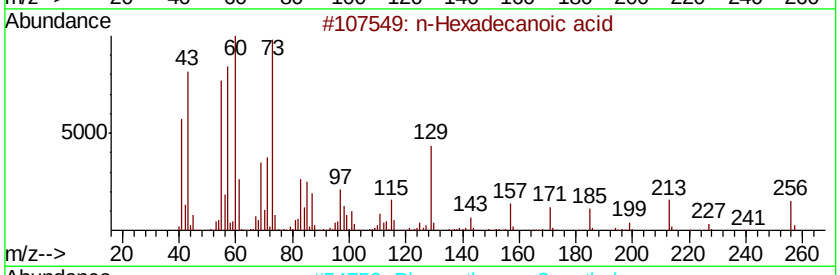
****

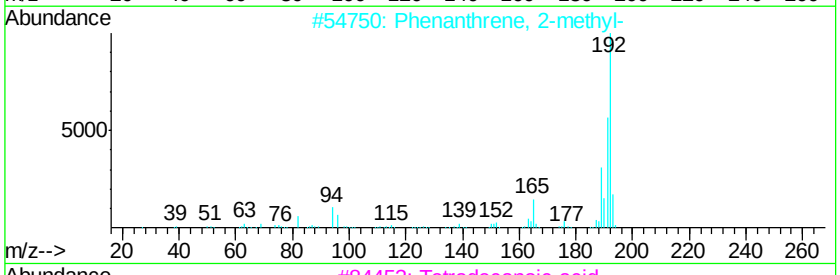
Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

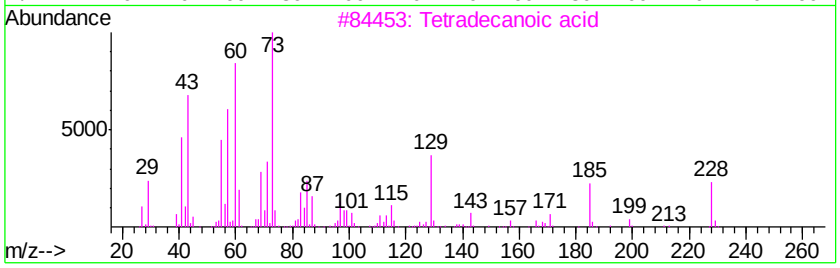
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.81	7.05 ng	393141	Phenanthrene-d10	11.28

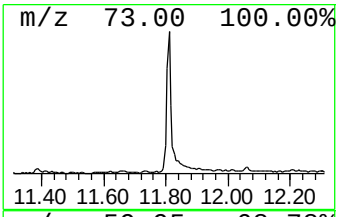
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	78
4	Tridecanoic acid	214	C13H26O2	000638-53-9	60
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	59

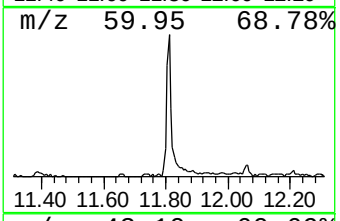


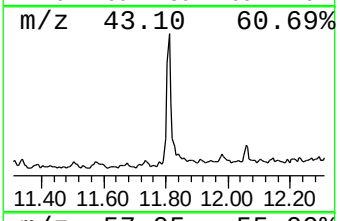


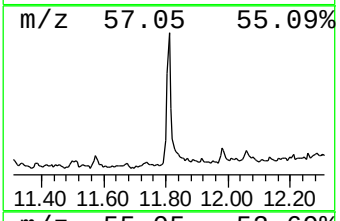


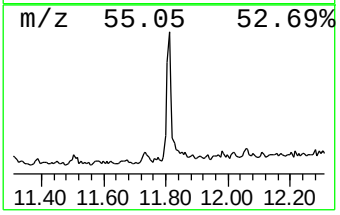












Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022020\
Data File : BF118987.D
Acq On : 21 Feb 2020 4:48
Operator : CG/JU
Sample : L1547-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MARCY-GREEN-BH-01-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

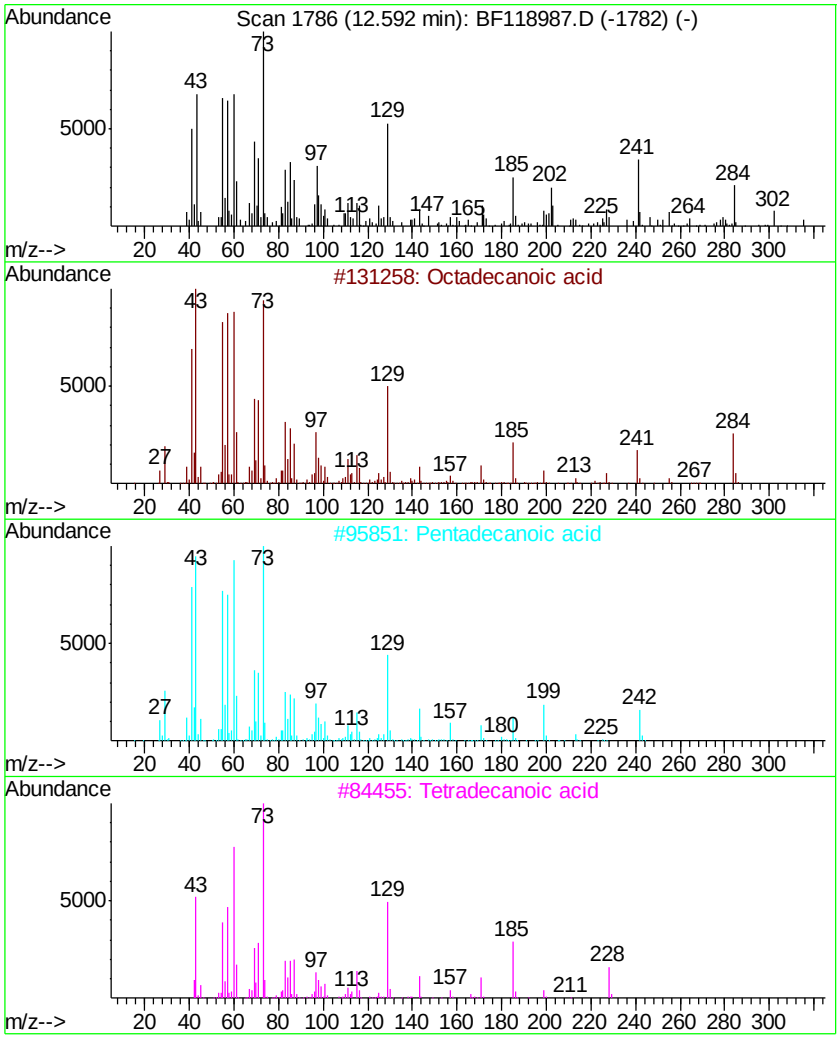
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

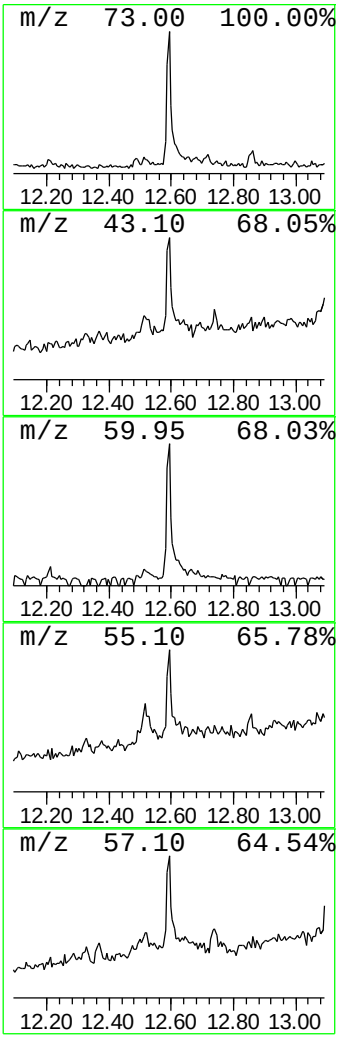
****

Peak Number 3 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.59	3.09 ng	172387	Phenanthrene-d10	11.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	n-Decanoic acid	172	C10H20O2	000334-48-5	46
5	Dodecanoic acid	200	C12H24O2	000143-07-7	30





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022020\
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Instrument : BNA_F
ClientSampleId : MARCY-GREEN-BH-01-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

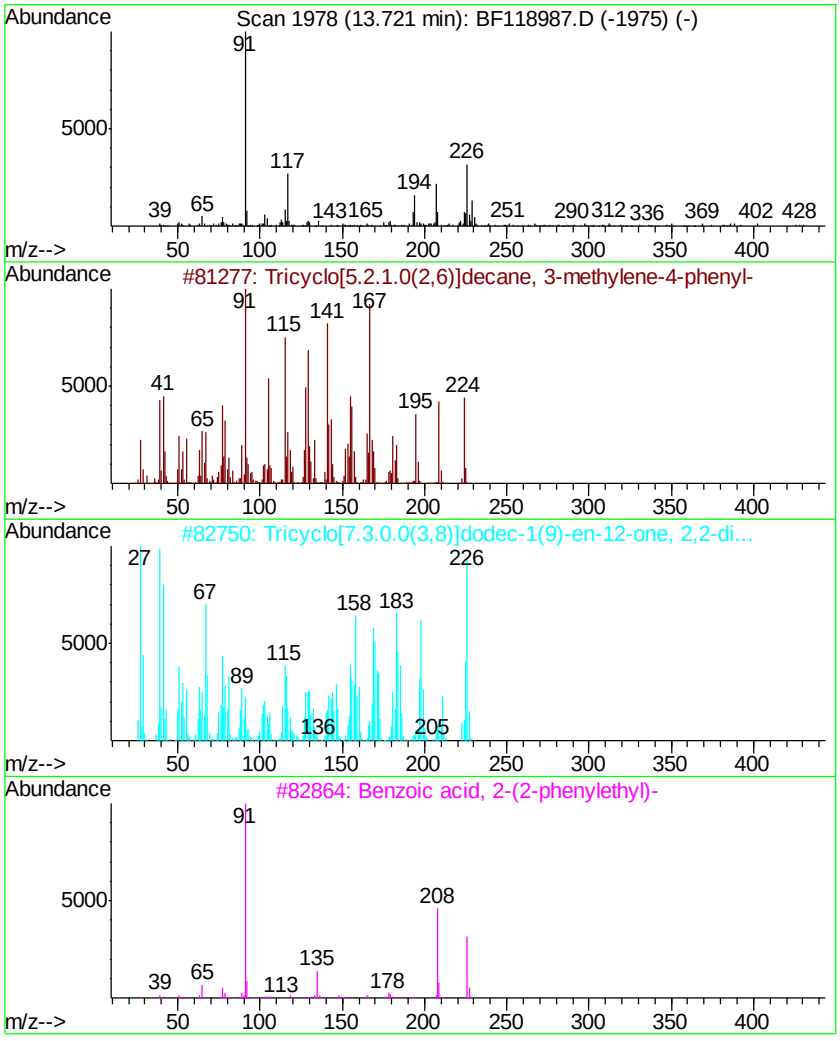
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

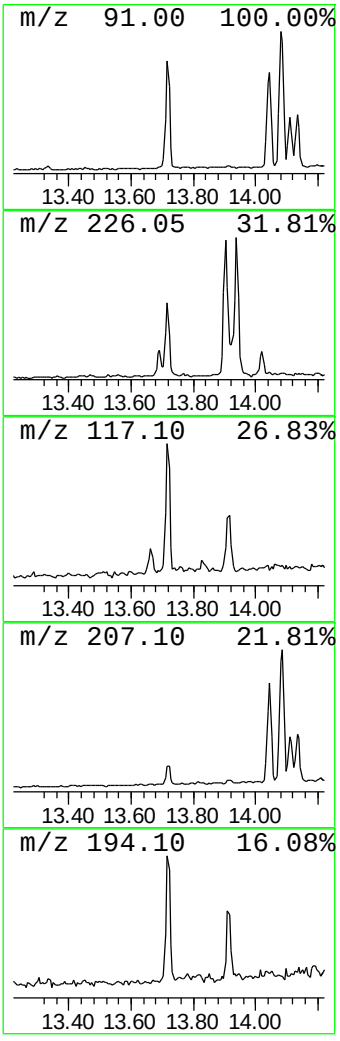
****

Peak Number 4 Tricyclo[5.2.1.0(2,6)]decan... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	2.67 ng	209182	Chrysene-d12	13.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricyclo[5.2.1.0(2,6)]decane, 3-...	224	C17H20	1000150-37-1	59
2	Tricyclo[7.3.0.0(3,8)]dodec-1(9)...	226	C14H14N2O	1000160-53-8	30
3	Benzoic acid, 2-(2-phenylethyl)-	226	C15H14O2	004890-85-1	25
4	2-Propanamine, N,N-dibenzyl	239	C17H21N	055578-14-8	10
5	Benzene, 1,1'-(1-ethyl-1,3-propa...	224	C17H20	000838-45-9	10





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022020\
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Instrument : BNA_F
ClientSampleId : MARCY-GREEN-BH-01-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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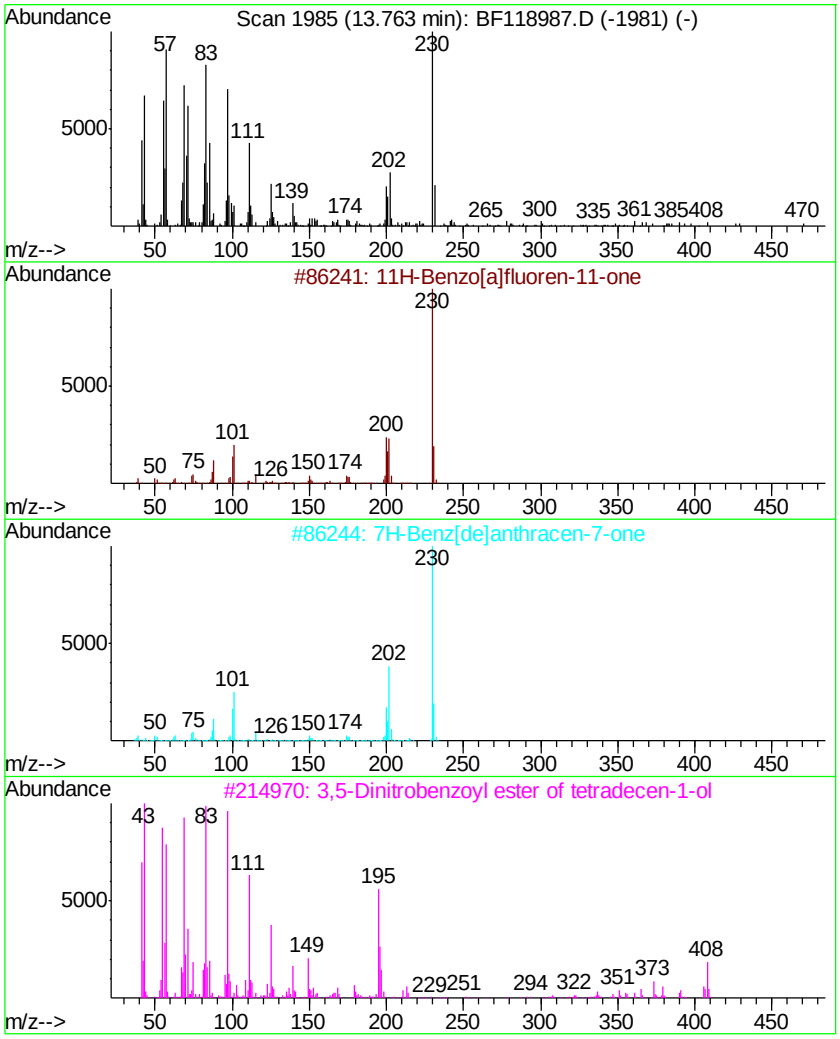
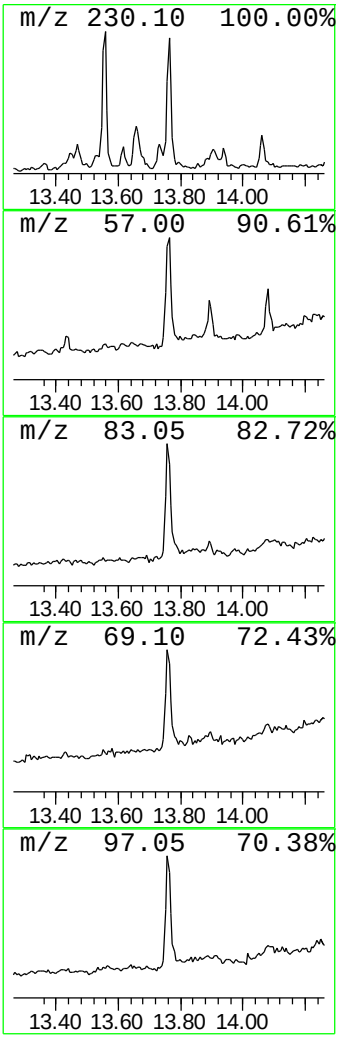
Peak Number 5 11H-Benzo[a]fluoren-11-one Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.76	4.94 ng	386746	Chrysene-d12	13.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	55
2	7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	38
3	3,5-Dinitrobenzoyl ester of tetr...	408	C21H32N2O6	094999-94-7	38
4	Ethane, 2,2-dichloro-1,1,1-trifl...	152	C2HCl2F3	000306-83-2	14
5	2,5-Diisopropyl-1,3,2-dithiabori...	202	C9H19BS2	110523-69-8	11





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Instrument : BNA_F
ClientSampleId : MARCY-GREEN-BH-01-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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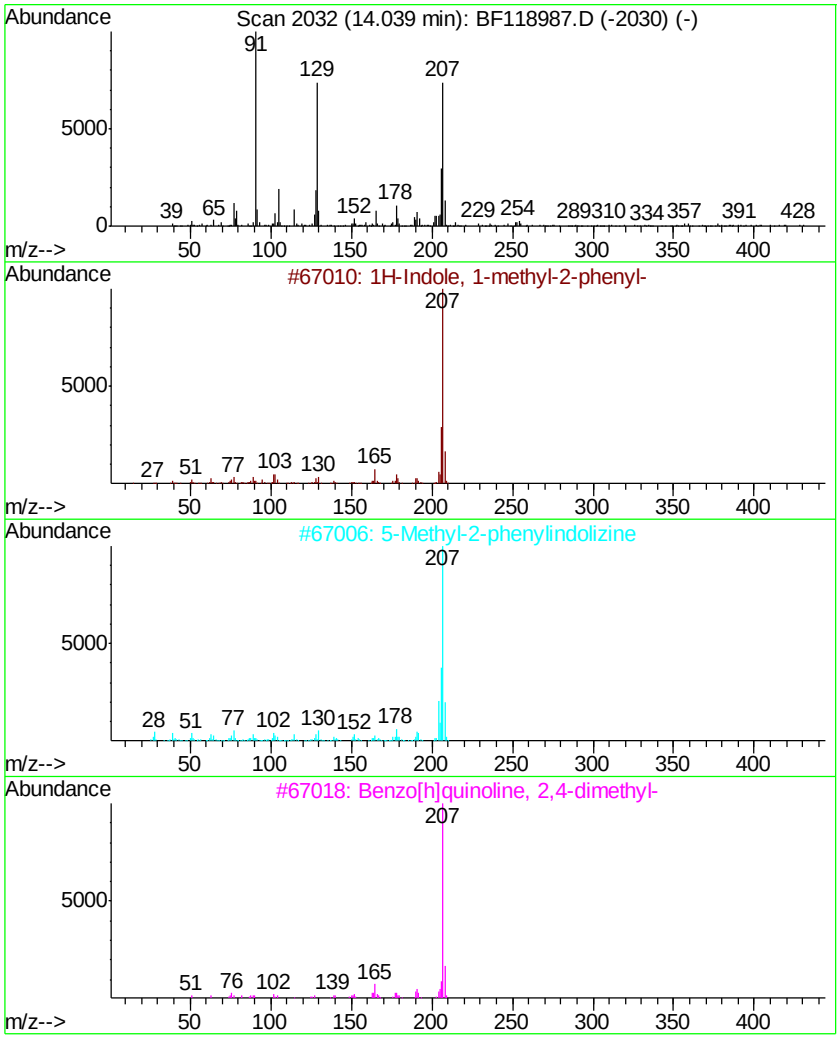
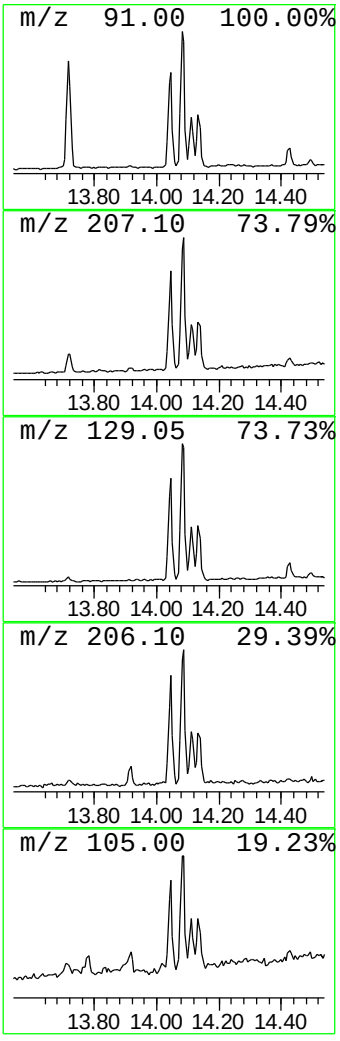
****

Peak Number 6 unknown14.04 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.04	3.56 ng	278391	Chrysene-d12	13.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	46
2	5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	45
3	Benzo[h]quinoline, 2,4-dimethyl-	207	C15H13N	000605-67-4	42
4	3-Methyl-2-phenylindole	207	C15H13N	010257-92-8	38
5	1H-Indole, 5-methyl-2-phenyl-	207	C15H13N	013228-36-9	38





Library Search Compound Report

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BNA_F
ClientSampleId :
MARCY-GREEN-BH-01-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.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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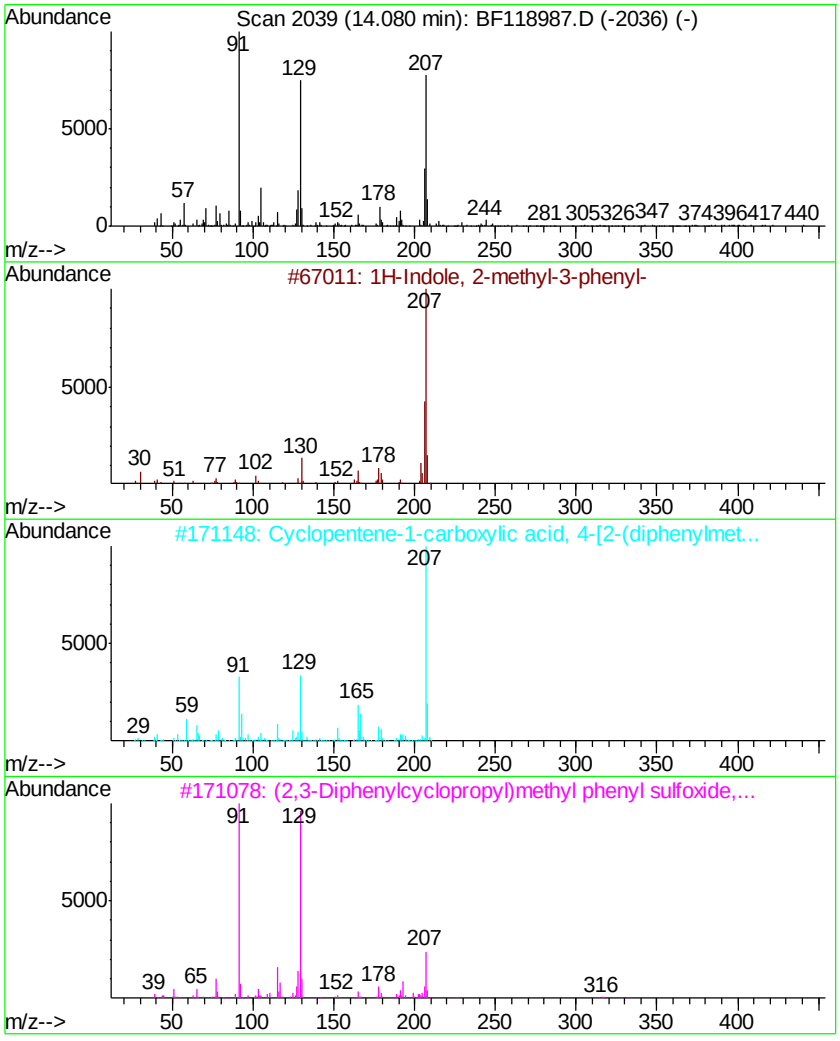
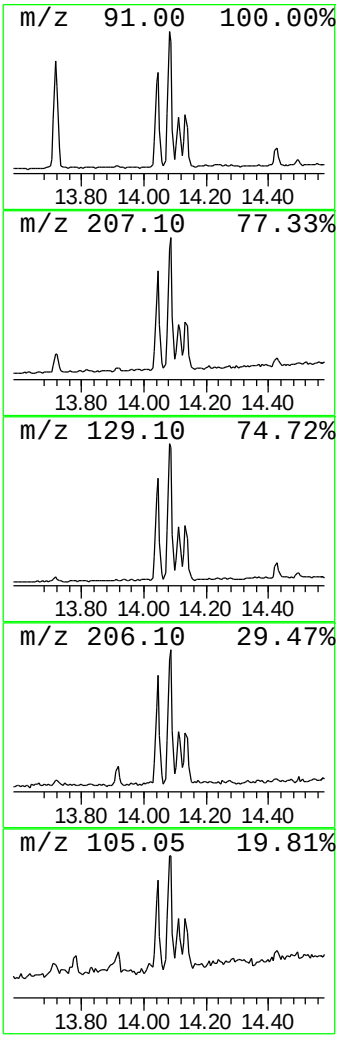
Peak Number 7 unknown14.08 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.08	5.58 ng	436699	Chrysene-d12	13.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indole, 2-methyl-3-phenyl-	207	C15H13N	004757-69-1	45
2	Cyclopentene-1-carboxylic acid, ...	332	C23H24O2	1000159-40-6	45
3	(2,3-Diphenylcyclopropyl)methyl ...	332	C22H20OS	131758-71-9	43
4	1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	38
5	1-Propene, 3-(2-cyclopentenyl)-2...	274	C21H22	1000154-23-3	38





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022020\
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Misc :
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Instrument : BNA_F
ClientSampleId : MARCY-GREEN-BH-01-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.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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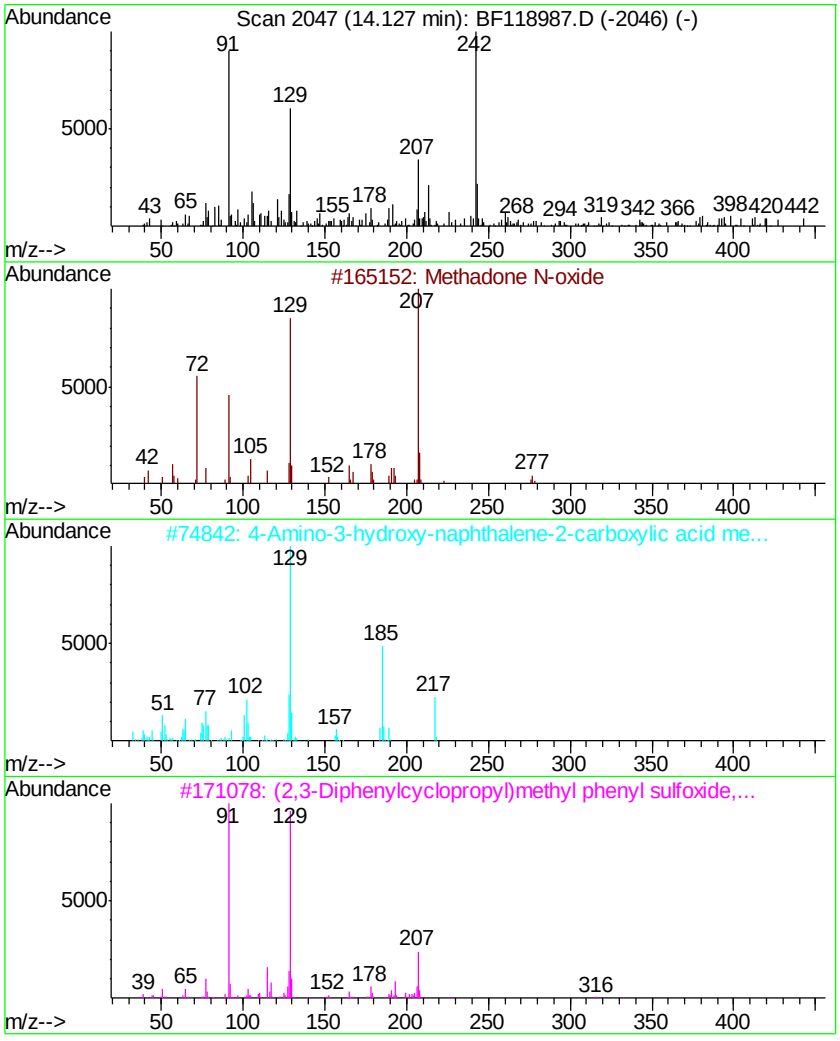
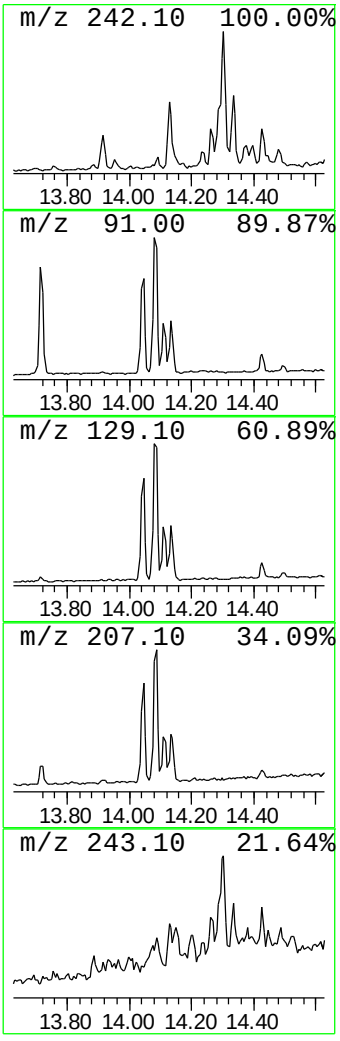
Peak Number 8 Methadone N-oxide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.13	2.63 ng	205655	Chrysene-d12	13.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methadone N-oxide	325	C21H27NO2	1000120-80-7	50
2	4-Amino-3-hydroxy-naphthalene-2-...	217	C12H11NO3	007399-72-6	43
3	(2,3-Diphenylcyclopropyl)methyl ...	332	C22H20OS	131758-71-9	41
4	1-Propene, 3-(2-cyclopentenyl)-2...	274	C21H22	1000154-23-3	40
5	1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	30





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022020\
Data File : BF118987.D
Acq On : 21 Feb 2020 4:48
Operator : CG/JU
Sample : L1547-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MARCY-GREEN-BH-01-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

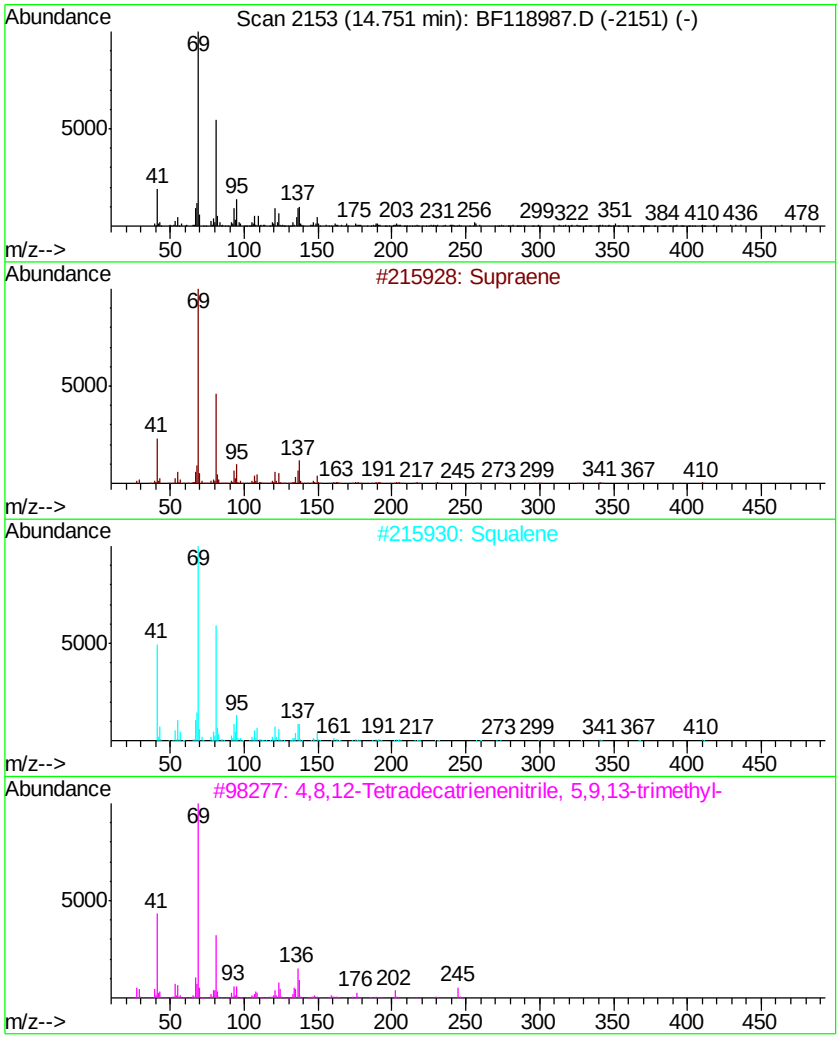
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

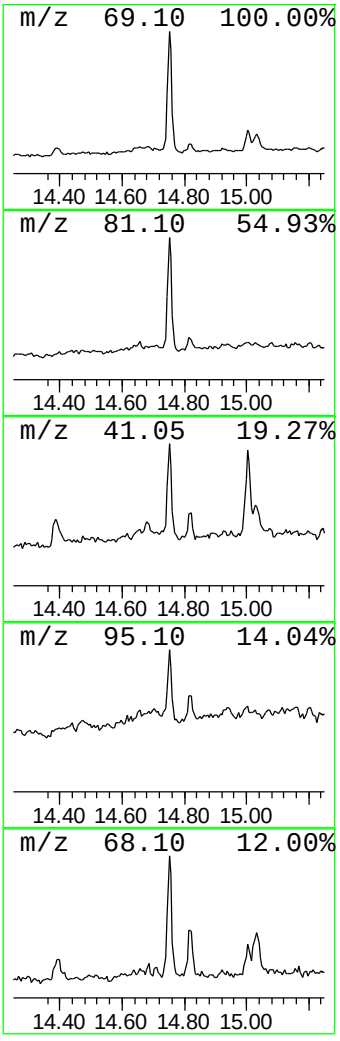
****

Peak Number 9 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.75	5.49 ng	343586	Perylene-d12	15.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	99
2	Squalene	410	C30H50	000111-02-4	90
3	4,8,12-Tetradecatrienenitrile, 5...	245	C17H27N	005981-31-7	64
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
5	Trideca-1,3,7,11-tetraene-1,1-di...	268	C18H24N2	1000159-88-9	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF022020\
Data File : BF118987.D
Acq On : 21 Feb 2020 4:48
Operator : CG/JU
Sample : L1547-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MARCY-GREEN-BH-01-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.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
n-Hexadecanoic acid	11.81	7.0	ng	393141	4	11.28	1115080	20.0
Octadecanoic acid	12.59	3.1	ng	172387	4	11.28	1115080	20.0
Tricyclo[5.2.1.0(...	13.72	2.7	ng	209182	5	13.92	1564510	20.0
11H-Benzo[a]fluor...	13.76	4.9	ng	386746	5	13.92	1564510	20.0
unknown14.04	14.04	3.6	ng	278391	5	13.92	1564510	20.0
unknown14.08	14.08	5.6	ng	436699	5	13.92	1564510	20.0
Methadone N-oxide	14.13	2.6	ng	205655	5	13.92	1564510	20.0
Supraene	14.75	5.5	ng	343586	6	15.35	1252270	20.0