LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030420\
Data File : BF119205.D
Acq On : 4 Mar 2020 20:22
Operator : CG/JU
Sample : L1770-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-1

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-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	5.375	556	559	584	rBV	1812627	2030146	93.41%	9.261%
2	6.398	730	733	750	rBV	1809340	1942078	89.36%	8.860%
3	6.739	788	791	799	rBV	826318	680213	31.30%	3.103%
4	6.898	814	818	826	rBV	2038841	1783599	82.07%	8.137%
5	7.304	883	887	898	rBV	1385658	1254214	57.71%	5.722%
6	8.022	1003	1009	1018	rBV	933043	819364	37.70%	3.738%
7	8.839	1143	1148	1156	rBV2	19446	32272	1.48%	0.147%
8	9.098	1187	1192	1195	rBV	2271893	2173298	100.00%	9.914%
9	9.180	1203	1206	1211	rBV3	35444	34637	1.59%	0.158%
10	9.492	1255	1259	1267	rVB	287175	285186	13.12%	1.301%
11	9.639	1281	1284	1288	rBV	51658	52059	2.40%	0.237%
12	9.710	1293	1296	1300	rVB	42917	35798	1.65%	0.163%
13	9.775	1303	1307	1311	rVV	911611	783864	36.07%	3.576%
14	9.804	1311	1312	1317	rVB	31572	28066	1.29%	0.128%
15	9.980	1338	1342	1346	rBV	27170	29995	1.38%	0.137%
16	10.204	1378	1380	1383	rVB2	39425	30093	1.38%	0.137%
17	10.322	1397	1400	1407	rVB	46625	48583	2.24%	0.222%
18	10.427	1412	1418	1422	rBV5	19517	26570	1.22%	0.121%
19	10.569	1438	1442	1452	rVB	1130713	1153096	53.06%	5.260%
20	10.674	1458	1460	1468	rVB4	43050	67230	3.09%	0.307%
21	10.869	1490	1493	1496	rBV3	20364	23920	1.10%	0.109%
22	11.121	1532	1536	1539	rBV2	37574	42583	1.96%	0.194%
23	11.157	1539	1542	1548	rVB	39491	42376	1.95%	0.193%
24	11.257	1556	1559	1562	rBV	777427	751463	34.58%	3.428%
25	11.280	1562	1563	1568	rVV	384584	284352	13.08%	1.297%
26	11.333	1569	1572	1576	rVB	97965	95246	4.38%	0.435%
27	11.498	1595	1600	1604	rBV3	45926	71069	3.27%	0.324%
28	11.551	1606	1609	1612	rVV	39303	32501	1.50%	0.148%
29	11.651	1622	1626	1629	rBV	94818	83480	3.84%	0.381%
30	11.716	1634	1637	1640	rBV3	21687	26985	1.24%	0.123%
31	11.763	1642	1645	1647	rBV	53210	47322	2.18%	0.216%
32	11.792	1647	1650	1655	rBV	223752	237497	10.93%	1.083%
33	11.874	1660	1664	1666	rBV	88423	88967	4.09%	0.406%
34	12.033	1688	1691	1693	rBV3	63168	59222	2.72%	0.270%

LSC Area Percent Report

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Acq On : 4 Mar 2020 20:22
Operator : CG/JU
Sample : L1770-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-1

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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

35	12.057	1693	1695	1699	rVB	35825	32270	1.48%	0.147%
36	12.310	1735	1738	1739	rBV	60247	52023	2.39%	0.237%
37	12.333	1739	1742	1743	rVV	289025	246442	11.34%	1.124%
38	12.351	1743	1745	1751	rVB3	292401	308331	14.19%	1.407%
39	12.404	1751	1754	1757	rBV2	33858	39717	1.83%	0.181%
40	12.439	1757	1760	1762	rBV2	44193	35087	1.61%	0.160%
41	12.474	1762	1766	1769	rBV	569651	510338	23.48%	2.328%
42	12.568	1780	1782	1788	rBV	69092	91258	4.20%	0.416%
43	12.621	1789	1791	1794	rVB3	27728	28477	1.31%	0.130%
44	12.704	1799	1805	1811	rBV	439922	537906	24.75%	2.454%
45	12.839	1824	1828	1831	rBV	2236821	1957746	90.08%	8.931%
46	12.921	1838	1842	1847	rBV3	43944	83235	3.83%	0.380%
47	13.098	1869	1872	1874	rVB2	50531	46985	2.16%	0.214%
48	13.133	1876	1878	1882	rVB2	43727	51889	2.39%	0.237%
49	13.257	1897	1899	1902	rBV2	41842	41044	1.89%	0.187%
50	13.739	1978	1981	1986	rBV3	151990	199559	9.18%	0.910%
51	13.898	2004	2008	2011	rBV2	844935	976925	44.95%	4.457%
52	13.927	2011	2013	2016	rVB	212980	167246	7.70%	0.763%
53	14.727	2145	2149	2154	rVB	792026	809674	37.26%	3.694%
54	15.333	2249	2252	2257	rVB	450143	526945	24.25%	2.404%

Sum of corrected areas: 21920441

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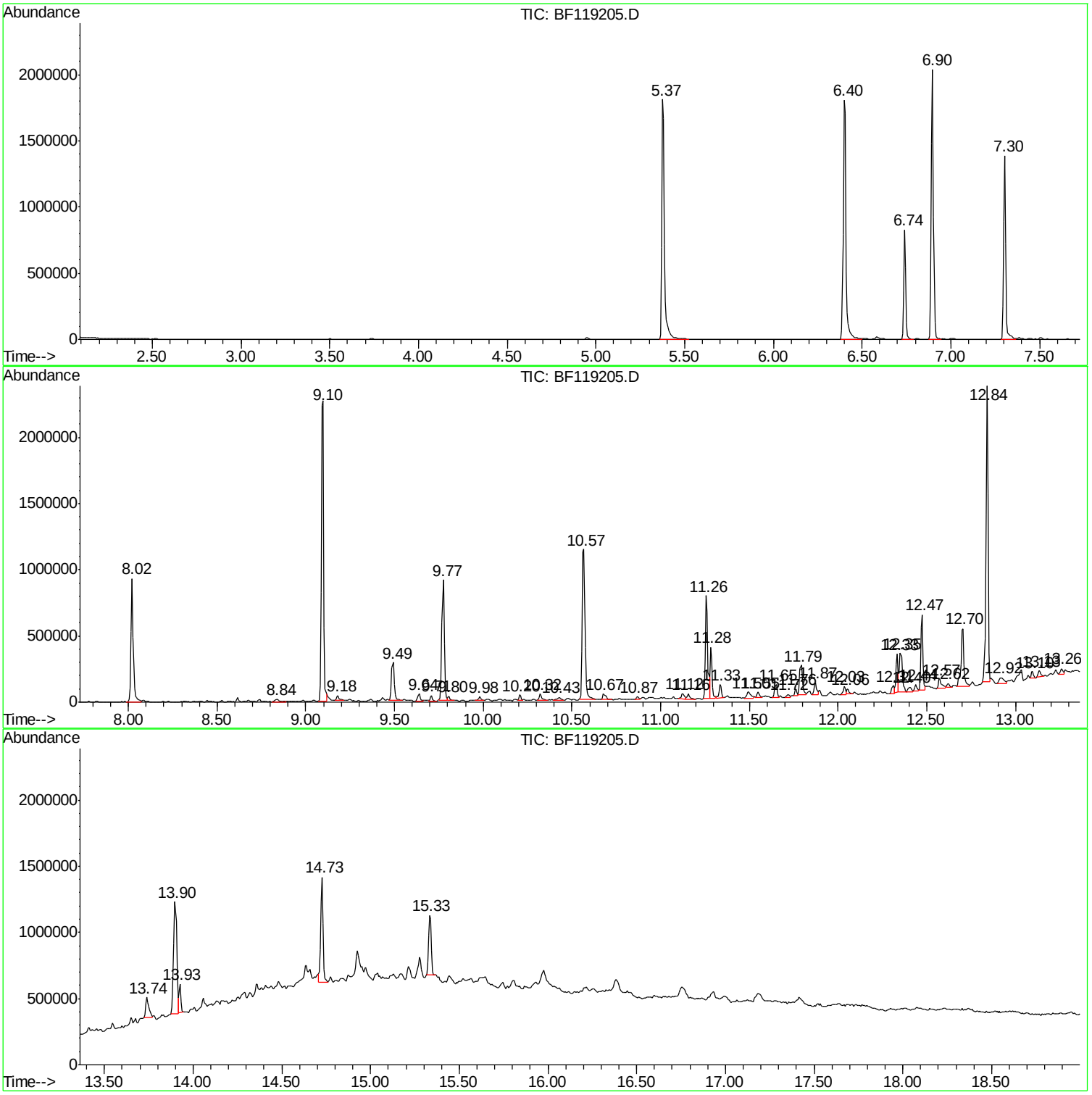
Operator : CG/JU
Sample : L1770-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C-1

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030420\
Data File : BF119205.D
Acq On : 4 Mar 2020 20:22
Operator : CG/JU
Sample : L1770-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-1

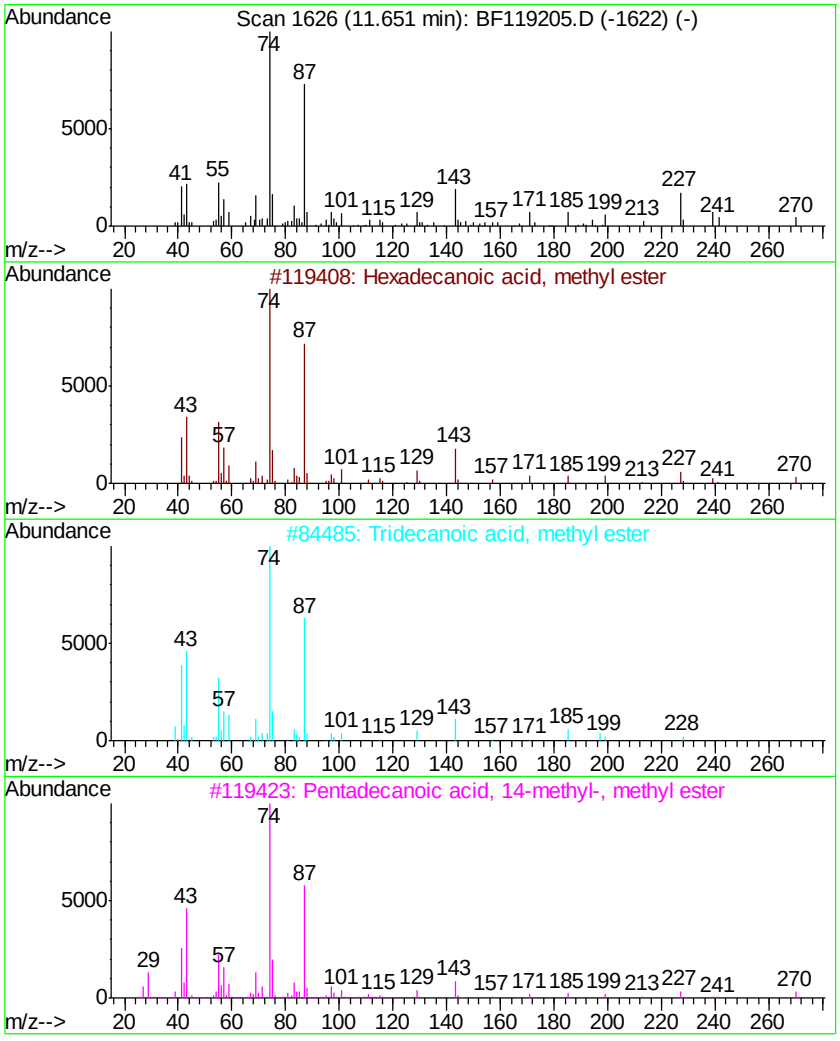
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

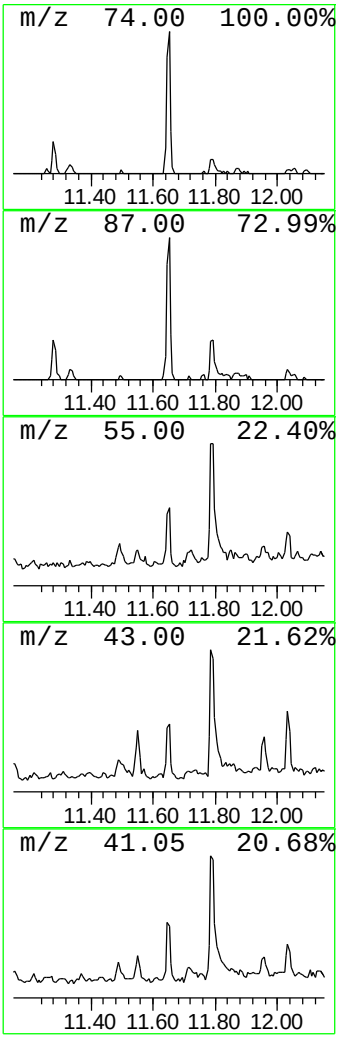
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.65	2.22 ng	83480	Phenanthrene-d10	11.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	96
2	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
3	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	81
4	Methyl 9-methyltetradecanoate	256	C16H32O2	213617-69-7	74
5	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	72





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030420\
Data File : BF119205.D
Acq On : 4 Mar 2020 20:22
Operator : CG/JU
Sample : L1770-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-1

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

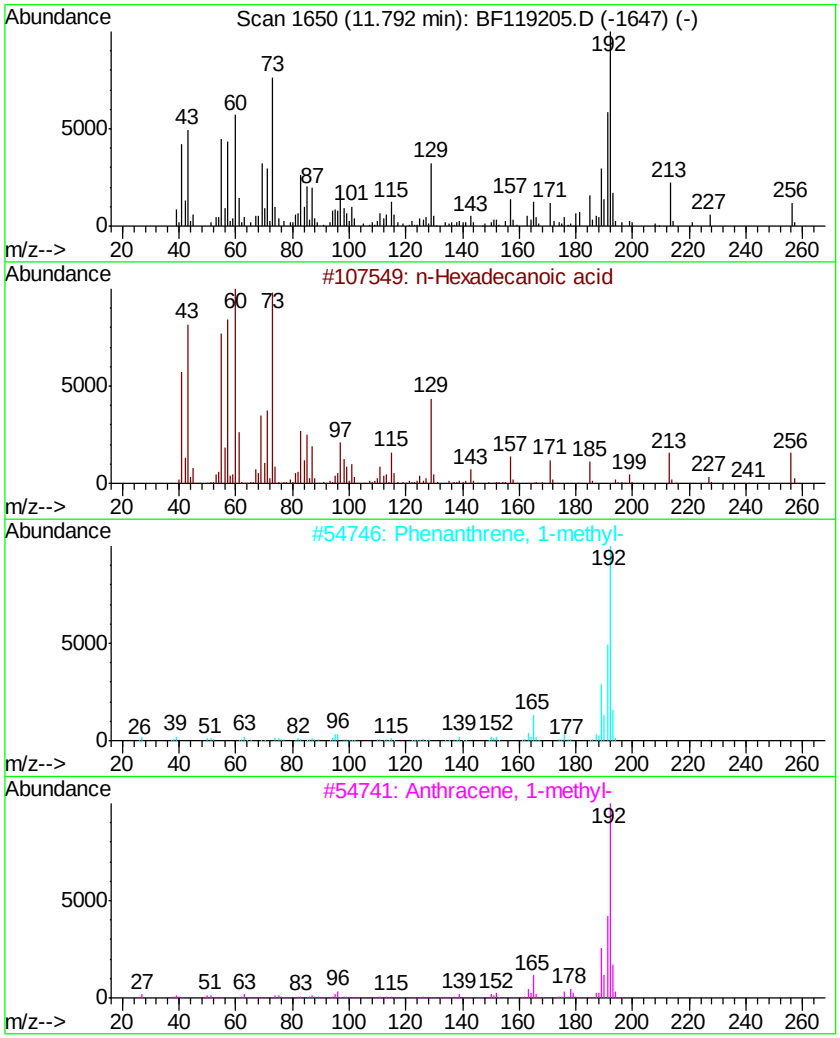
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

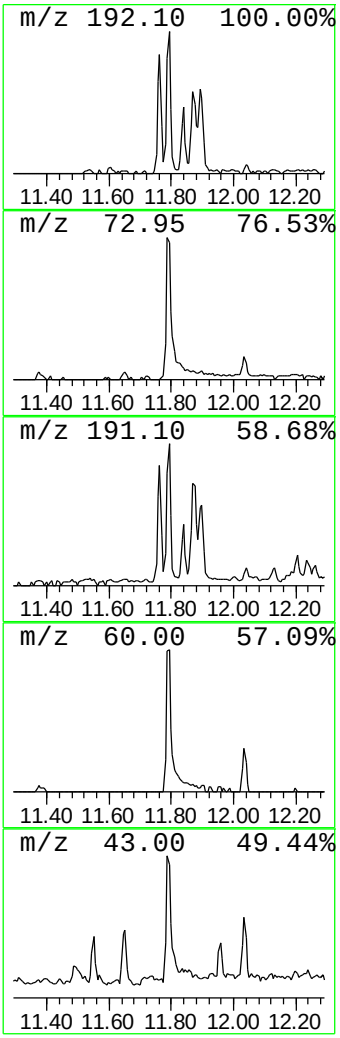
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	6.32 ng	237497	Phenanthrene-d10	11.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	93
3	Anthracene, 1-methyl-	192	C15H12	000610-48-0	86
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	86
5	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	86





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030420\
Data File : BF119205.D
Acq On : 4 Mar 2020 20:22
Operator : CG/JU
Sample : L1770-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-1

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

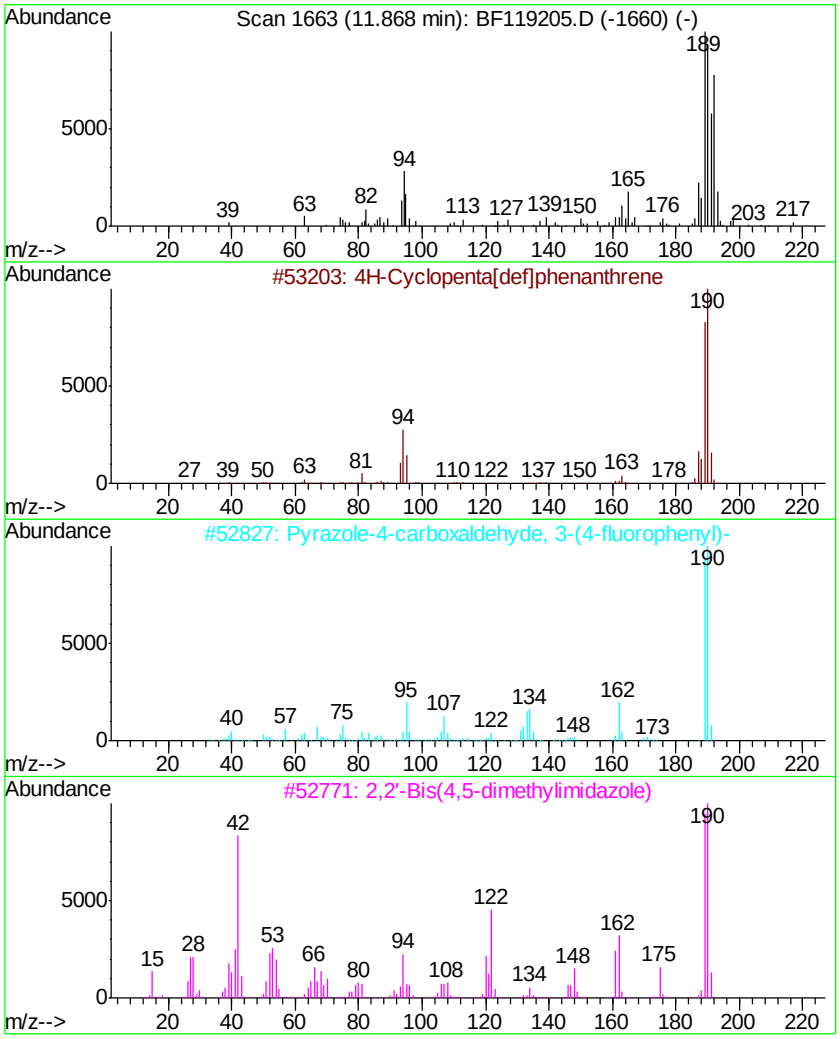
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

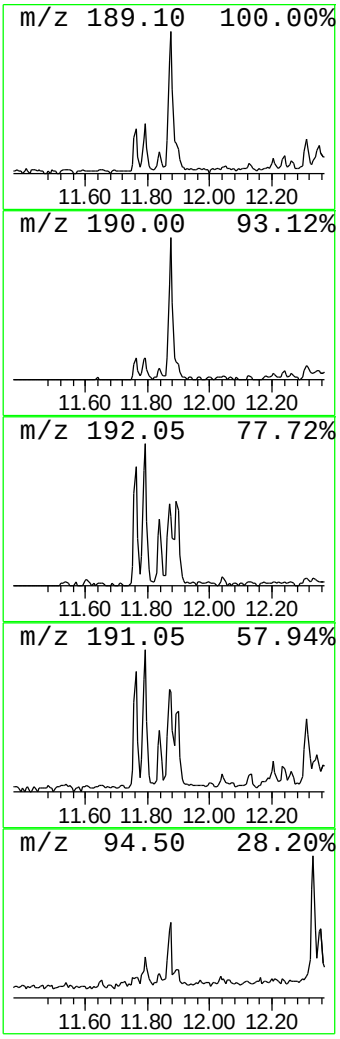
****

Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	2.37 ng	88967	Phenanthrene-d10	11.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	58
2	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	43
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	28
4	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	25
5	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	25





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030420\
Data File : BF119205.D
Acq On : 4 Mar 2020 20:22
Operator : CG/JU
Sample : L1770-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-1

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

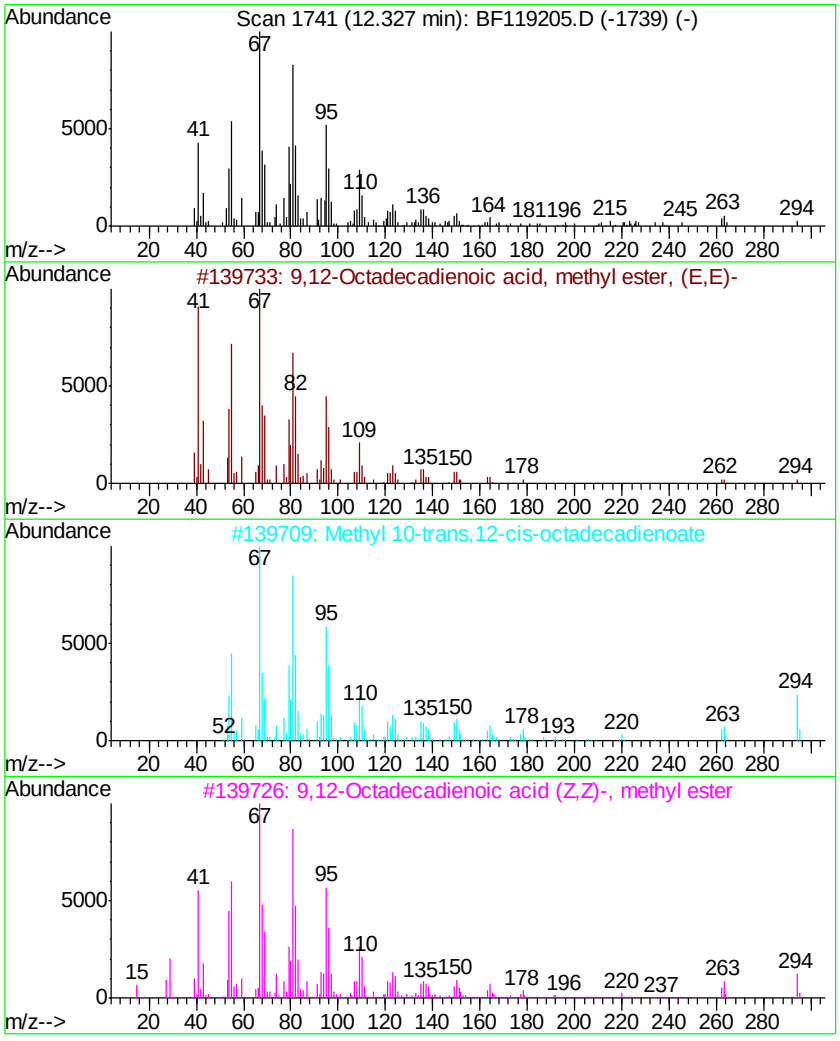
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

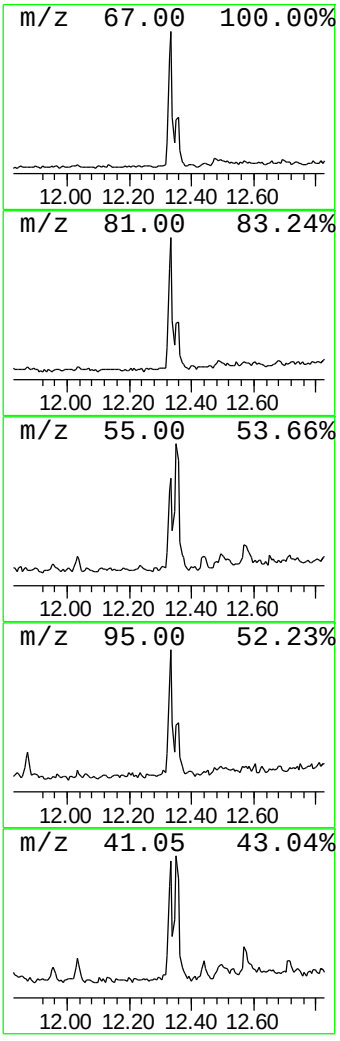
****

Peak Number 5 9,12-Octadecadienoic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.33	6.56 ng	246442	Phenanthrene-d10	11.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	98
3	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	98
4	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	98
5	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	97





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Operator : CG/JU
Sample : L1770-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-1

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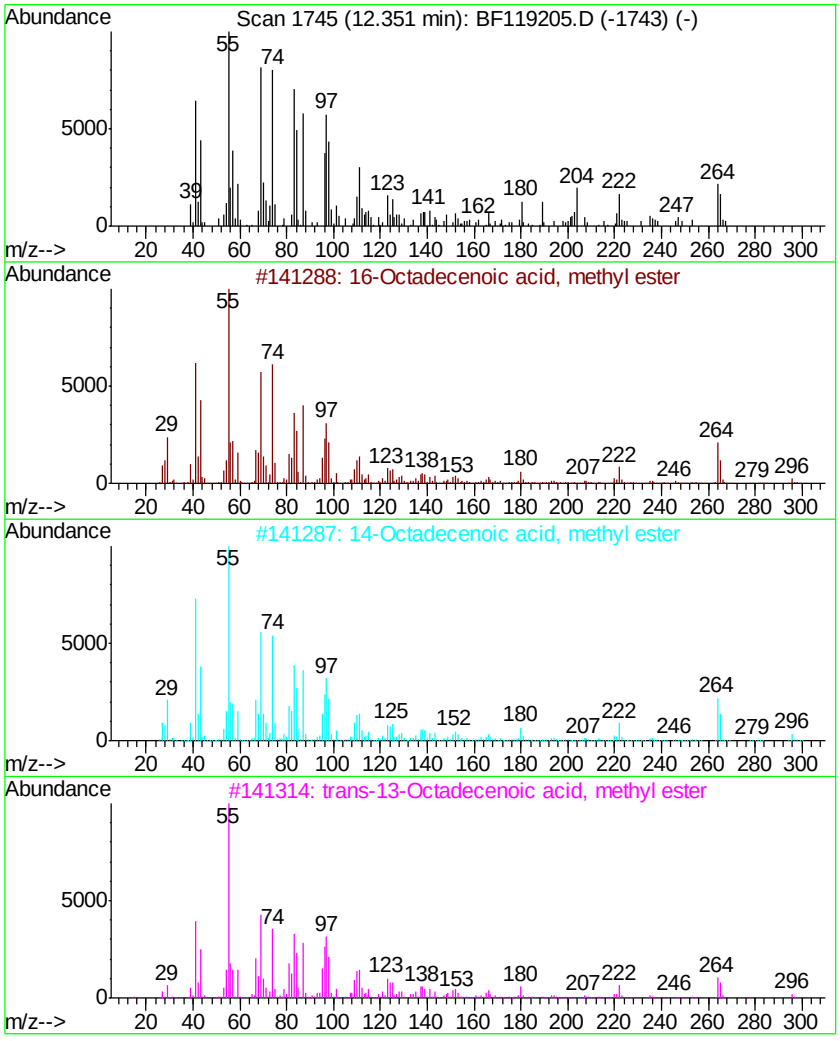
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

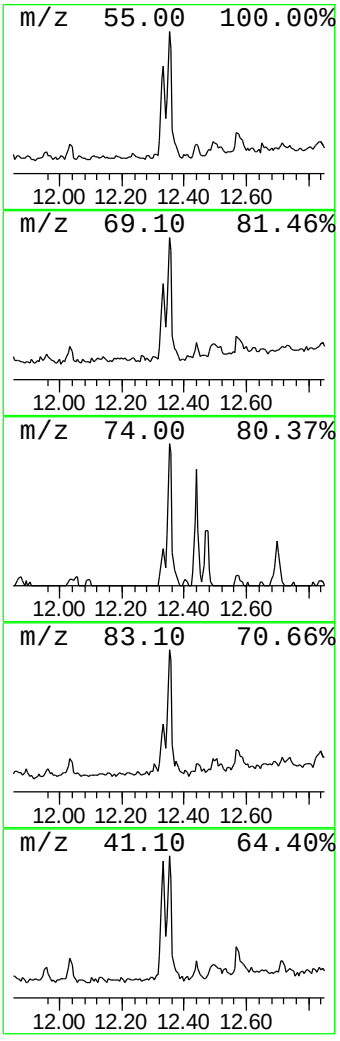
****

Peak Number 6 16-Octadecenoic acid, methy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.35	8.21 ng	308331	Phenanthrene-d10	11.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	70
2	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	58
3	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	49
4	Oleic Acid	282	C18H34O2	000112-80-1	46
5	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	46





Library Search Compound Report

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Operator : CG/JU
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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-1

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

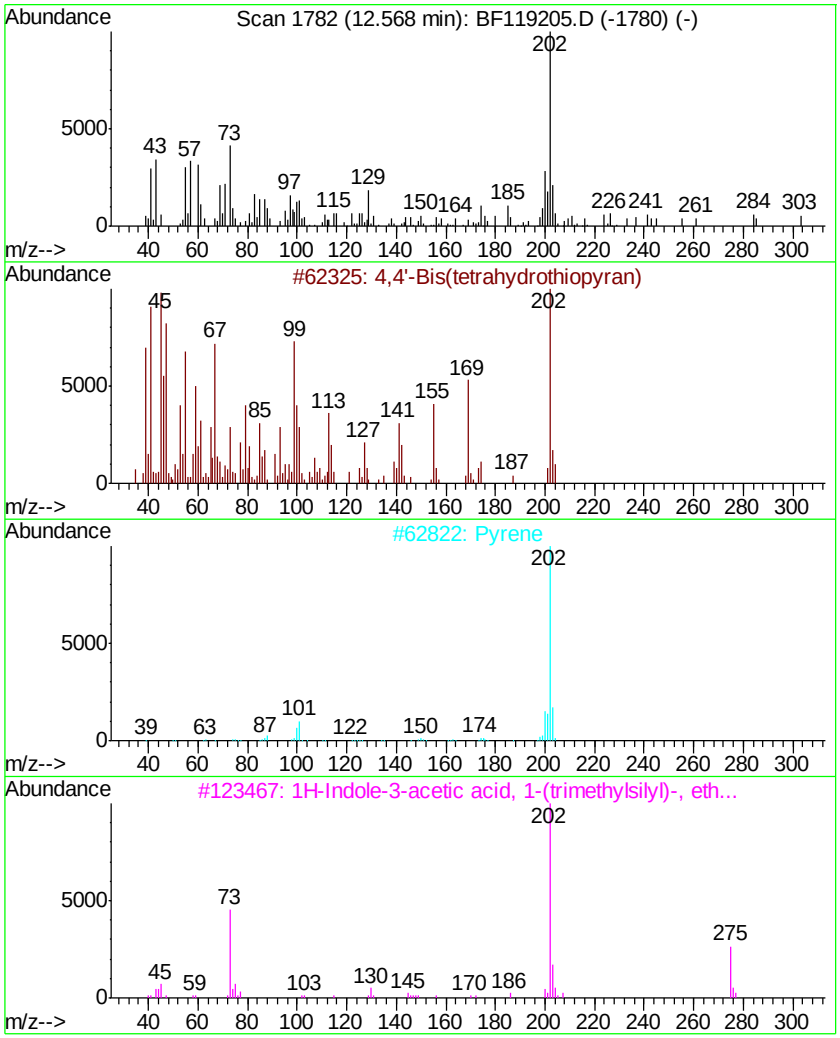
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

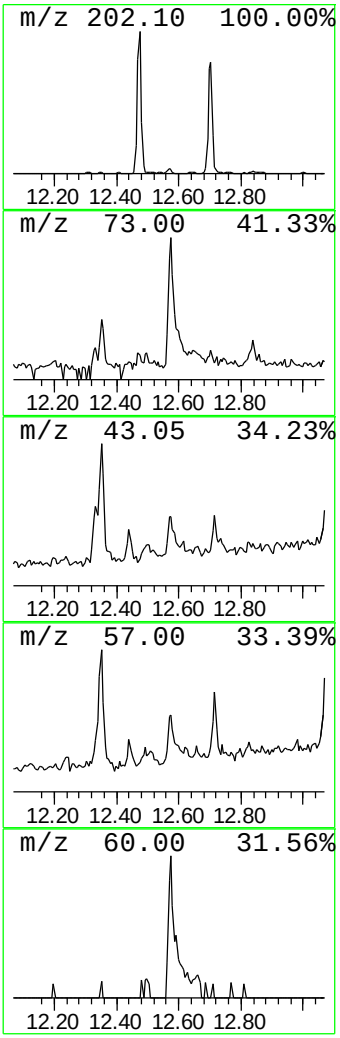
****

Peak Number 7 4,4'-Bis(tetrahydrothiopyran) Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	2.43 ng	91258	Phenanthrene-d10	11.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4'-Bis(tetrahydrothiopyran)	202	C10H18S2	116196-83-9	86
2	Pyrene	202	C16H10	000129-00-0	52
3	1H-Indole-3-acetic acid, 1-(trim...	275	C15H21NO2Si	074367-38-7	47
4	Fluoranthene	202	C16H10	000206-44-0	47
5	Di-1H-pyrrol-1-yl-isopropenylsilane	202	C11H14N2Si	1000306-57-7	46





Library Search Compound Report

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Sample : L1770-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-1

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

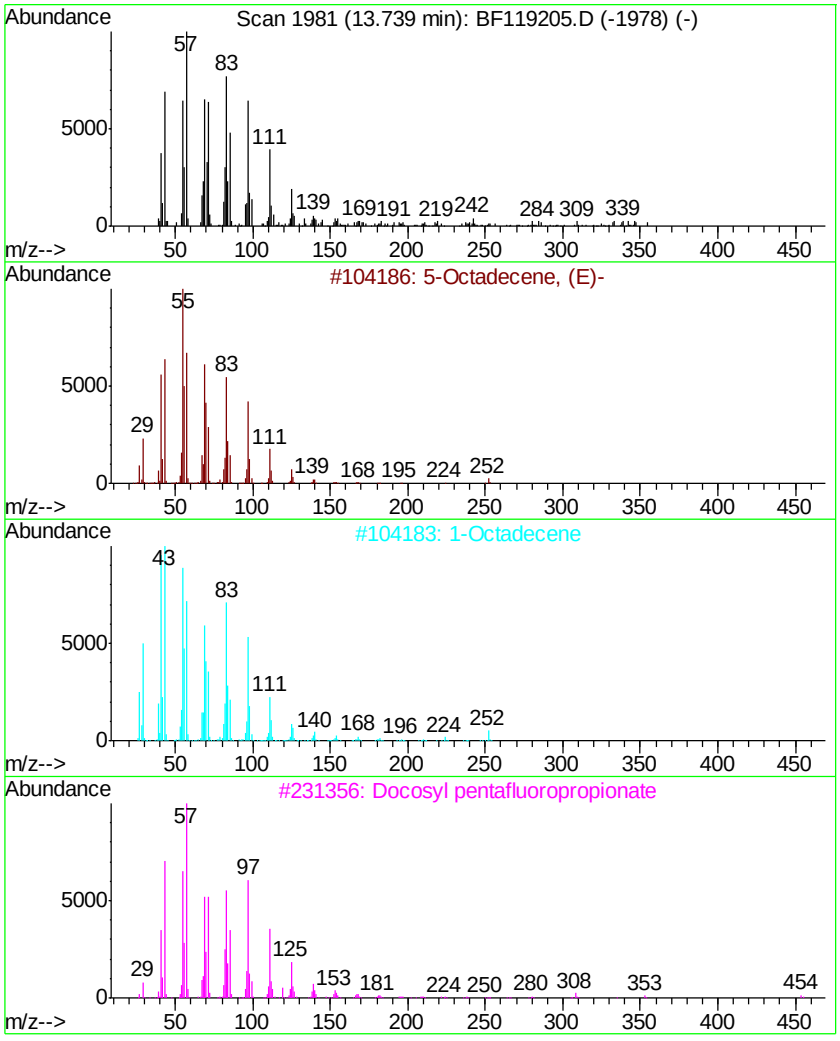
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

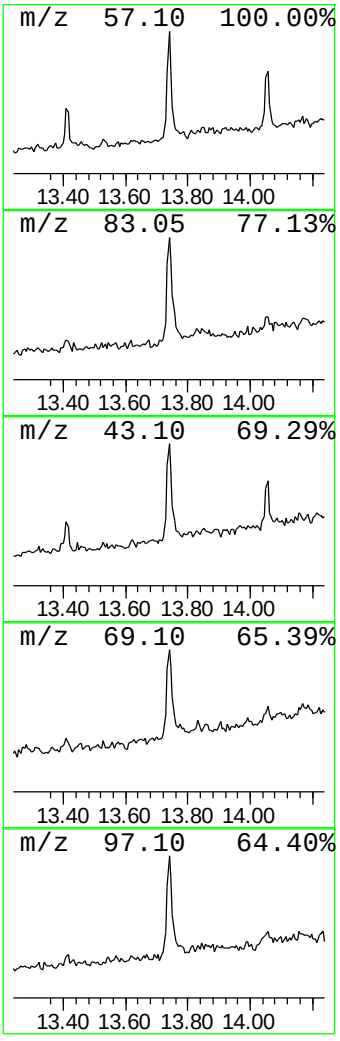
****

Peak Number 8 5-Octadecene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	4.09 ng	199559	Chrysene-d12	13.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	93
2	1-Octadecene	252	C18H36	000112-88-9	93
3	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
4	Oxalic acid, octadecyl propyl ester	384	C23H44O4	1000309-27-0	91
5	5-Eicosene, (E)-	280	C20H40	074685-30-6	90





Library Search Compound Report

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Data File : BF119205.D
Acq On : 4 Mar 2020 20:22
Operator : CG/JU
Sample : L1770-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-1

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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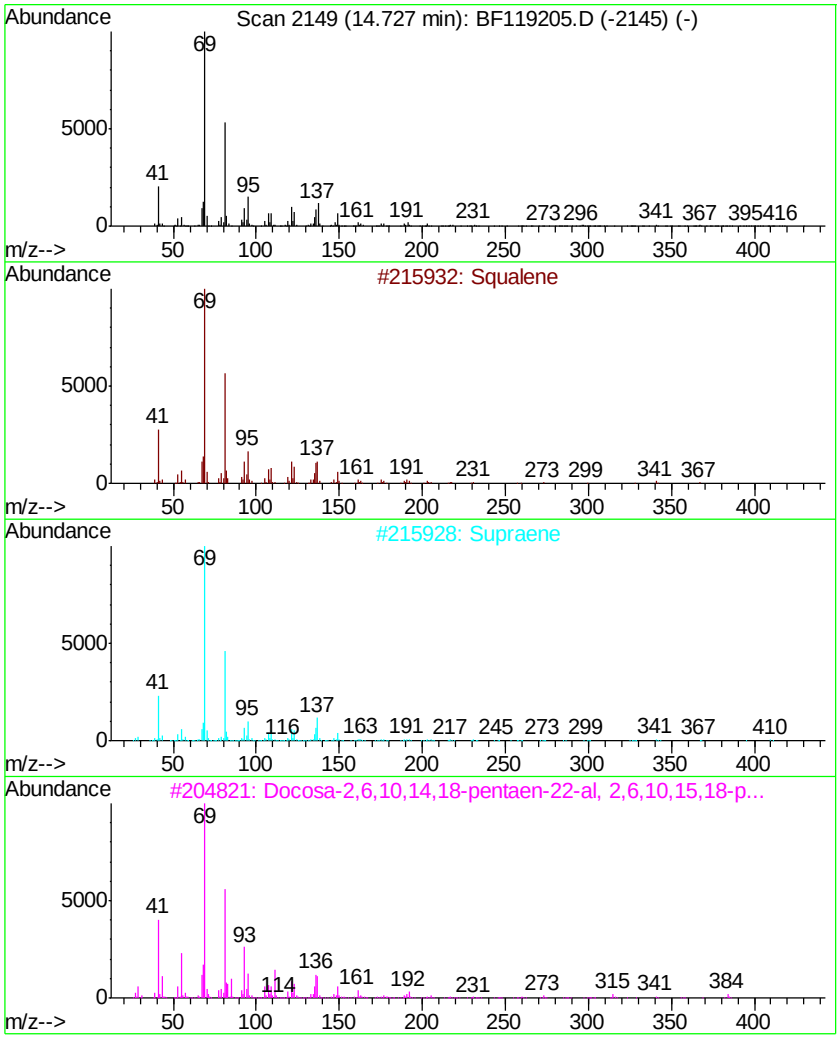
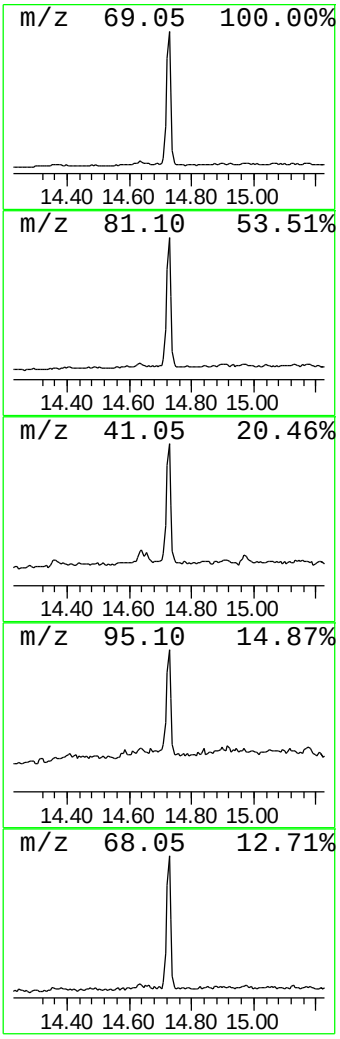
Peak Number 9 Squalene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	30.73 ng	809674	Perylene-d12	15.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	94
2	Supraene	410	C30H50	007683-64-9	91
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
4	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	78
5	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	78





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030420\
Data File : BF119205.D
Acq On : 4 Mar 2020 20:22
Operator : CG/JU
Sample : L1770-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-1

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
Hexadecanoic acid...	11.65	2.2	ng	83480	4	11.26	751463	20.0
n-Hexadecanoic acid	11.79	6.3	ng	237497	4	11.26	751463	20.0
4H-Cyclopenta[def...	11.87	2.4	ng	88967	4	11.26	751463	20.0
9,12-Octadecadien...	12.33	6.6	ng	246442	4	11.26	751463	20.0
16-Octadecenoic a...	12.35	8.2	ng	308331	4	11.26	751463	20.0
4,4'-Bis(tetrahyd...	12.57	2.4	ng	91258	4	11.26	751463	20.0
5-Octadecene, (E)-	13.74	4.1	ng	199559	5	13.90	976925	20.0
Squalene	14.73	30.7	ng	809674	6	15.34	526945	20.0