LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040319\
Data File : BF113553.D
Acq On : 3 Apr 2019 19:47
Operator : JU/SJ
Sample : K2213-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S9C(2-10)COMP

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-BF040319.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	5.304	542	547	571	rBV	3344240	3416137	90.32%	9.611%
2	6.340	718	723	739	rBV	3285756	3566840	94.30%	10.035%
3	6.457	739	743	747	rBV	3432359	3520906	93.09%	9.906%
4	6.687	778	782	791	rBV	882736	773035	20.44%	2.175%
5	6.840	804	808	812	rBV	2857507	2765682	73.12%	7.781%
6	7.251	873	878	881	rBV	2264192	2164988	57.24%	6.091%
7	7.969	996	1000	1010	rBV	926324	915483	24.20%	2.576%
8	9.045	1178	1183	1187	rBV	3857629	3782363	100.00%	10.642%
9	9.439	1247	1250	1255	rBV	221627	190367	5.03%	0.536%
10	9.722	1294	1298	1310	rVB	1029169	902090	23.85%	2.538%
11	10.510	1428	1432	1447	rBV	2043624	2084131	55.10%	5.864%
12	11.204	1546	1550	1553	rBV	970327	848729	22.44%	2.388%
13	11.228	1553	1554	1557	rVV	78667	46865	1.24%	0.132%
14	11.280	1558	1563	1568	rVB	55775	57482	1.52%	0.162%
15	11.739	1638	1641	1651	rBV3	138411	231800	6.13%	0.652%
16	12.298	1732	1736	1741	rBV2	36611	54408	1.44%	0.153%
17	12.345	1741	1744	1747	rVB2	37397	37997	1.00%	0.107%
18	12.416	1752	1756	1760	rBV	346328	320593	8.48%	0.902%
19	12.527	1771	1775	1779	rBV2	222915	278529	7.36%	0.784%
20	12.639	1790	1794	1798	rVB	369117	350046	9.25%	0.985%
21	12.792	1815	1820	1822	rBV	3281461	3356424	88.74%	9.443%
22	12.816	1822	1824	1827	rVB2	97575	85846	2.27%	0.242%
23	12.951	1844	1847	1849	rBV3	39044	49943	1.32%	0.141%
24	13.039	1857	1862	1864	rBV2	29806	44305	1.17%	0.125%
25	13.074	1864	1868	1876	rVB2	53676	88345	2.34%	0.249%
26	13.486	1935	1938	1942	rVB	59368	59383	1.57%	0.167%
27	13.592	1953	1956	1958	rBV	44865	40449	1.07%	0.114%
28	13.639	1962	1964	1970	rVB2	39613	53745	1.42%	0.151%
29	13.721	1970	1978	1990	rBV4	160772	603100	15.95%	1.697%
30	13.839	1993	1998	2001	rVV2	1046745	1165031	30.80%	3.278%
31	13.863	2001	2002	2006	rVB	207842	145703	3.85%	0.410%
32	14.010	2024	2027	2030	rBV	103263	91836	2.43%	0.258%
33	14.316	2076	2079	2082	rVB	130140	132068	3.49%	0.372%
34	14.610	2125	2129	2132	rBV	221099	229989	6.08%	0.647%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040319\
Data File : BF113553.D
Acq On : 3 Apr 2019 19:47
Operator : JU/SJ
Sample : K2213-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S9C(2-10)COMP

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-BF040319.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.674	2138	2140	2143	rVB	74103	58217	1.54%	0.164%
36	14.851	2167	2170	2173	rBV	212257	286933	7.59%	0.807%
37	14.921	2178	2182	2185	rVV	263932	275670	7.29%	0.776%
38	15.133	2215	2218	2224	rBV	110940	155120	4.10%	0.436%
39	15.192	2225	2228	2231	rVV	120123	161596	4.27%	0.455%
40	15.251	2233	2238	2250	rVB2	665551	1304937	34.50%	3.671%
41	15.668	2305	2309	2315	rVB	298306	428204	11.32%	1.205%
42	16.127	2383	2387	2398	rVB	216529	418146	11.06%	1.176%

Sum of corrected areas: 35543461

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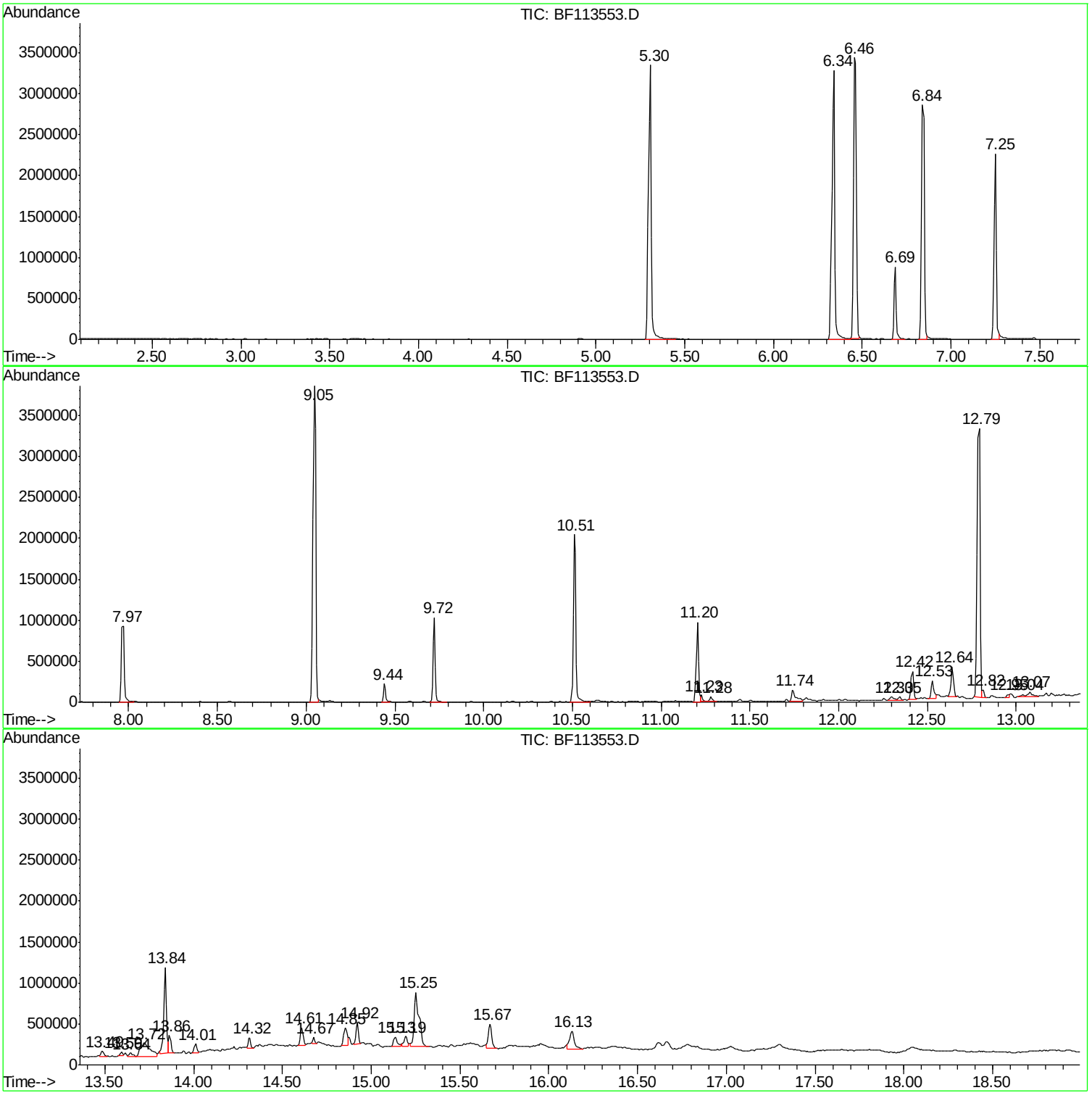
Instrument :
BNA_F
ClientSampleId :
S9C(2-10)COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.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\BF040319\
Data File : BF113553.D
Acq On : 3 Apr 2019 19:47
Operator : JU/SJ
Sample : K2213-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S9C(2-10)COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.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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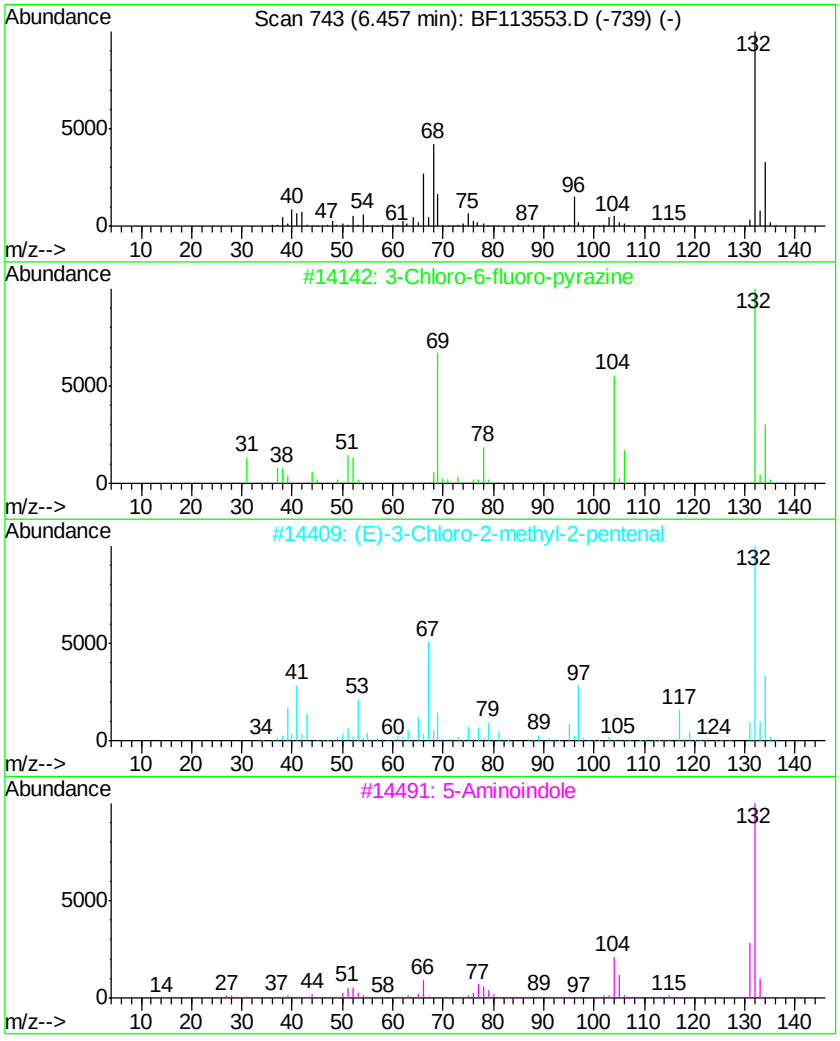
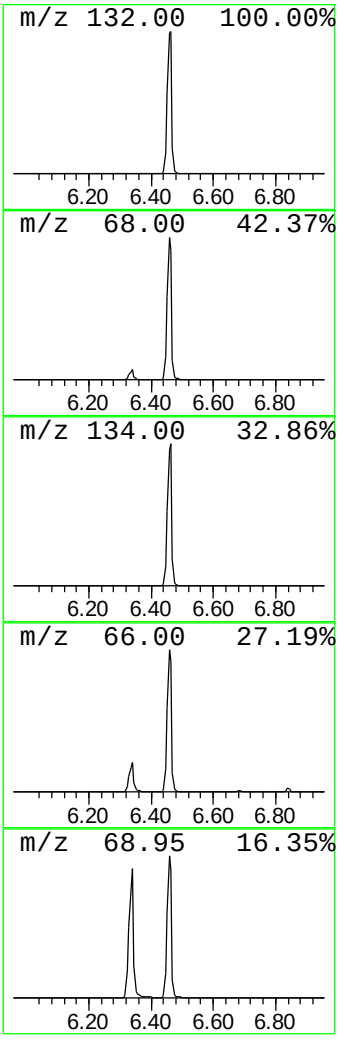
Peak Number 1 unknown6.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	91.09 ng	3520910	1,4-Dichlorobenzene-d4	6.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Amphetaminil	250	C17H18N2	017590-01-1	10





Library Search Compound Report

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Data File : BF113553.D
Acq On : 3 Apr 2019 19:47
Operator : JU/SJ
Sample : K2213-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S9C(2-10)COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

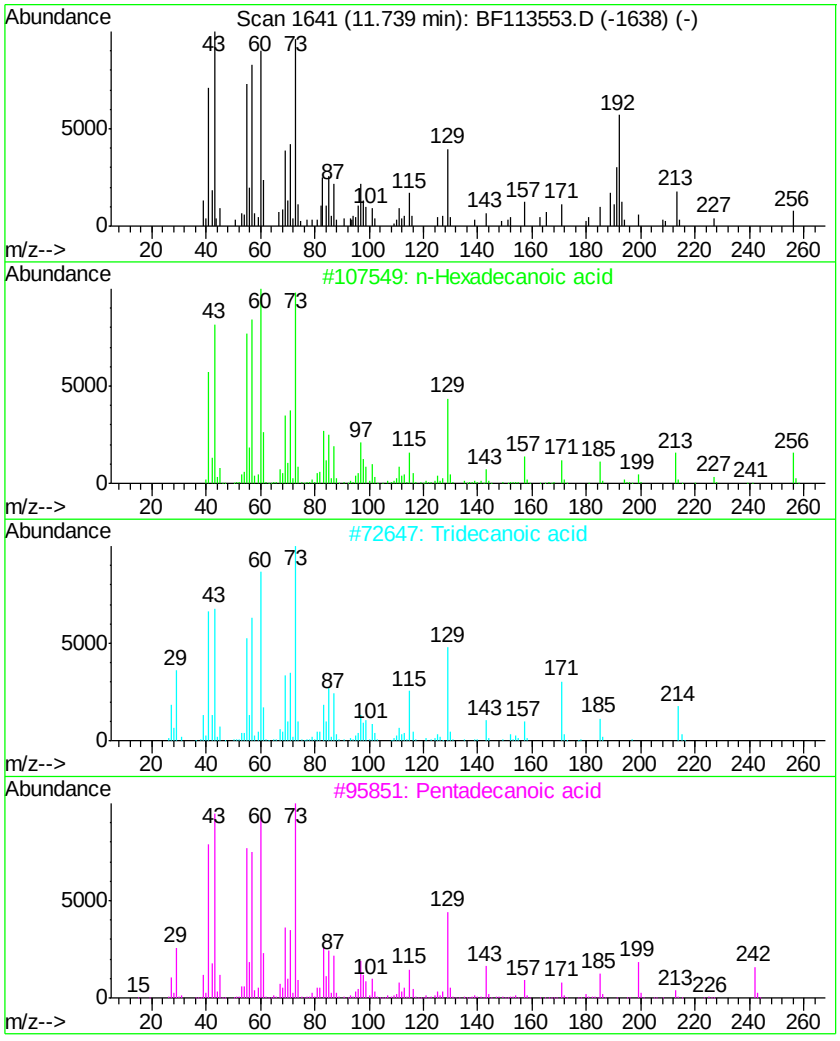
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

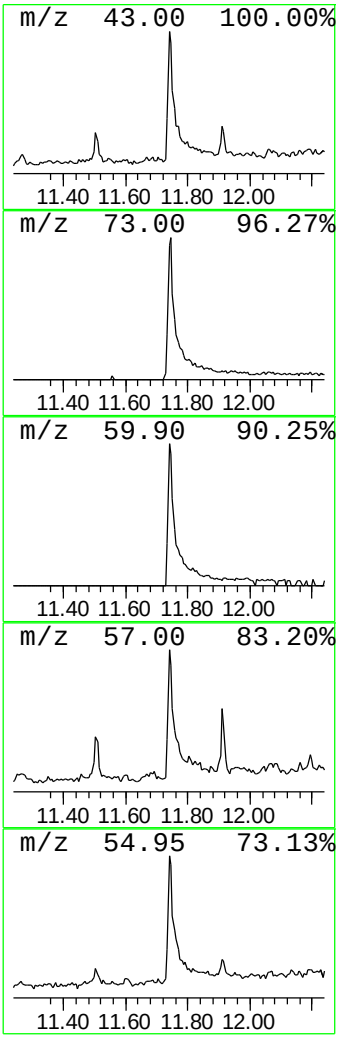
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.74	5.46 ng	231800	Phenanthrene-d10	11.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Undecanoic acid	186	C11H22O2	000112-37-8	50





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040319\
Data File : BF113553.D
Acq On : 3 Apr 2019 19:47
Operator : JU/SJ
Sample : K2213-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S9C(2-10)COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

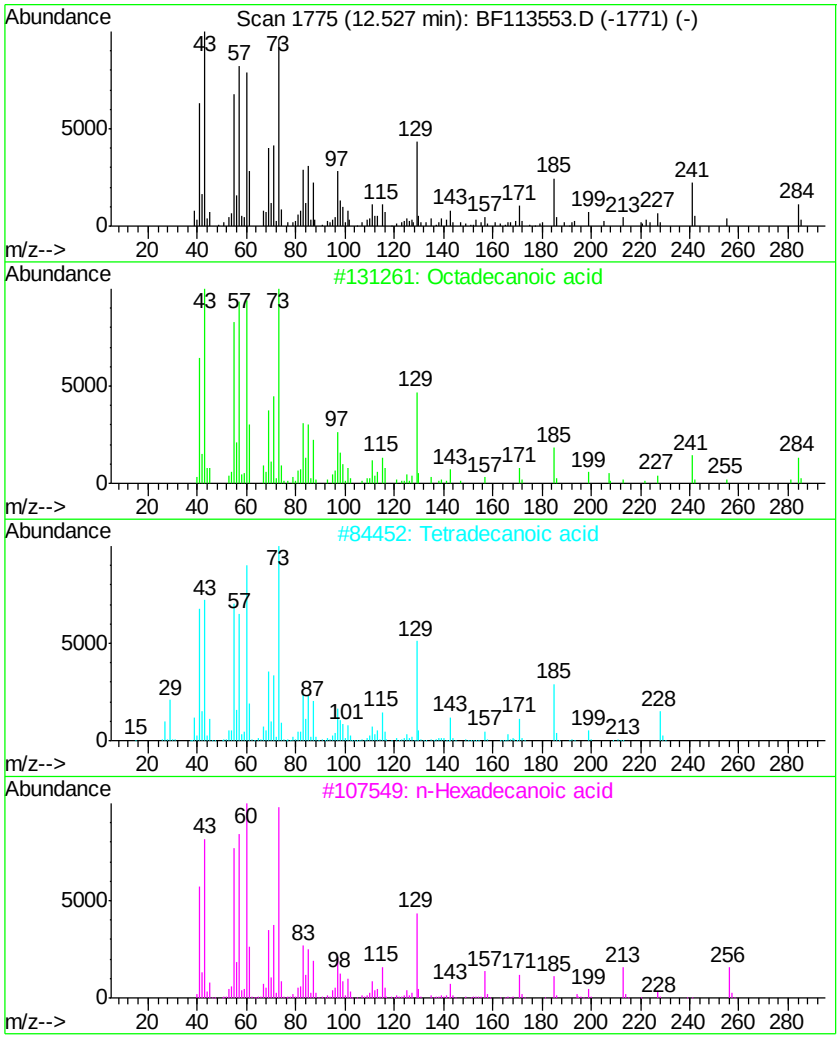
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

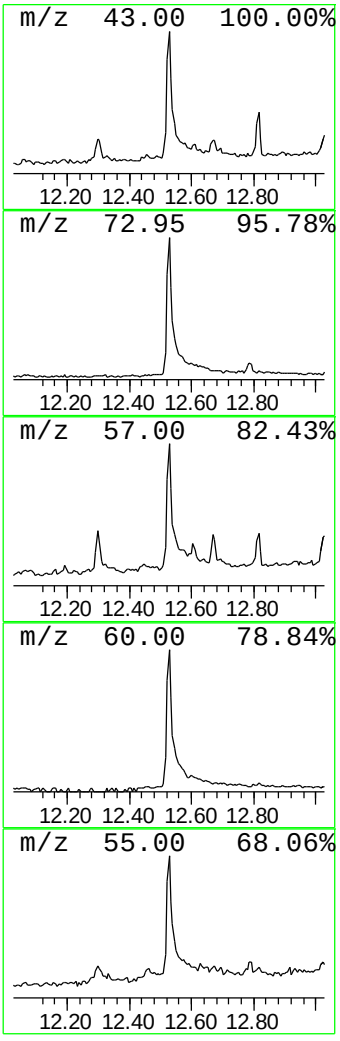
****

Peak Number 4 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.53	4.78 ng	278529	Chrysene-d12	13.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
4	Undecanoic acid	186	C11H22O2	000112-37-8	74
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040319\
Data File : BF113553.D
Acq On : 3 Apr 2019 19:47
Operator : JU/SJ
Sample : K2213-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S9C(2-10)COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

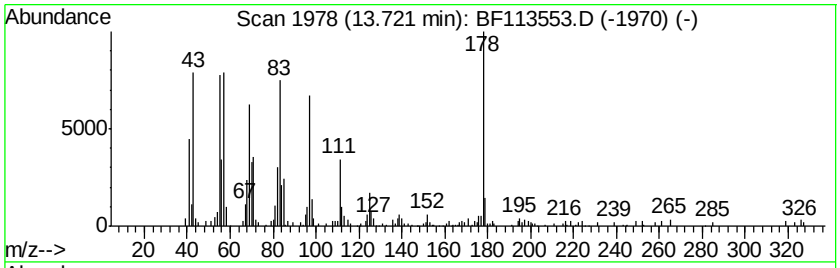
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

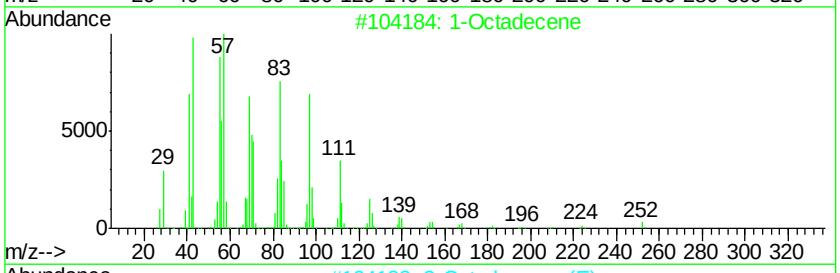
****

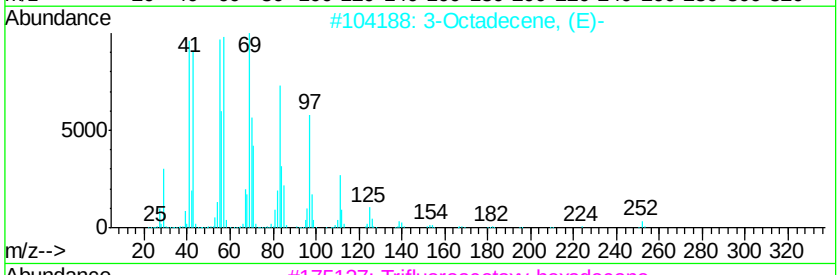
Peak Number 5 1-Octadecene Concentration Rank 3

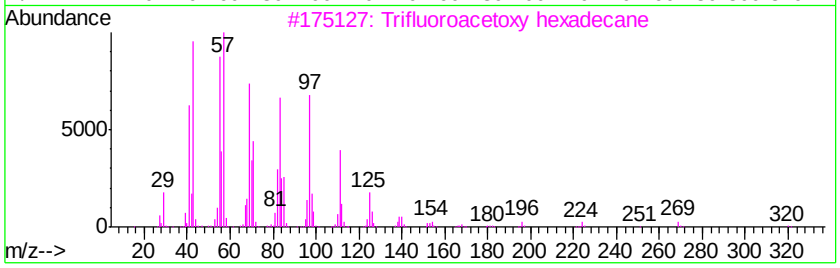
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	10.35 ng	603100	Chrysene-d12	13.84

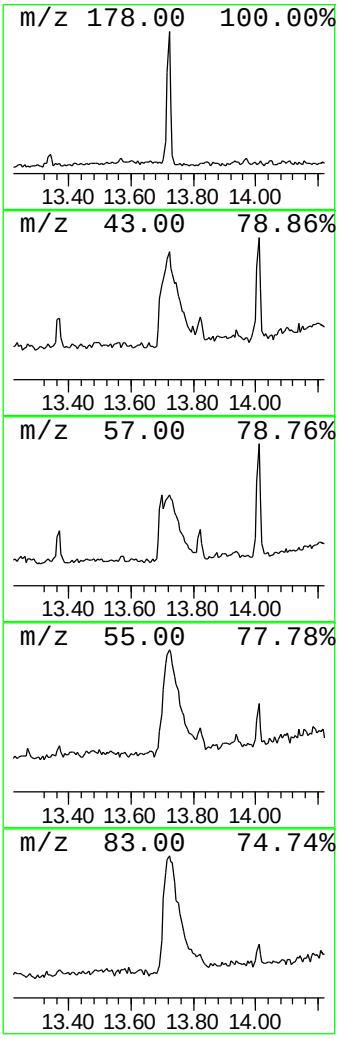
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene	252	C18H36	000112-88-9	95
2	3-Octadecene, (E)-	252	C18H36	007206-19-1	94
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	89
4	1-Heneicosanol	312	C21H44O	015594-90-8	86
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	86











Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040319\
Data File : BF113553.D
Acq On : 3 Apr 2019 19:47
Operator : JU/SJ
Sample : K2213-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S9C(2-10)COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

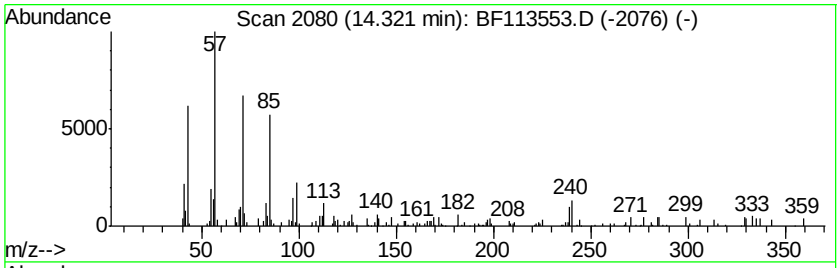
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

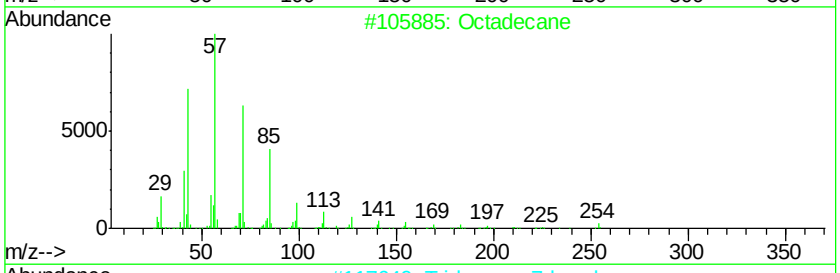
****

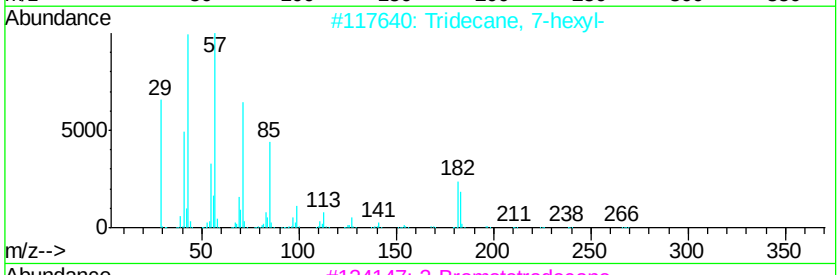
Peak Number 6 Octadecane Concentration Rank 10

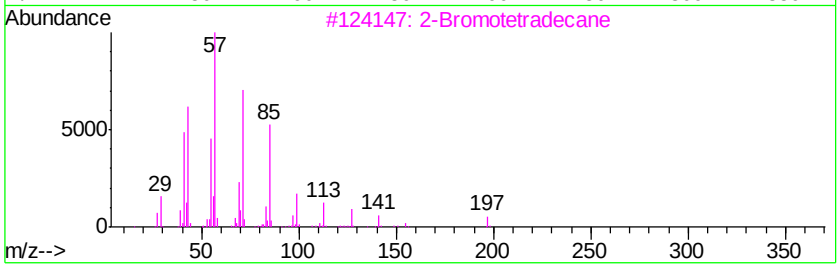
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.32	2.27 ng	132068	Chrysene-d12	13.84

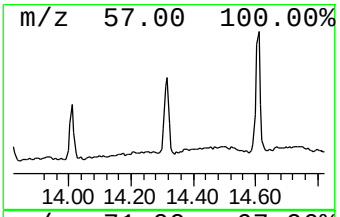
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	93
2	Tridecane, 7-hexyl-	268	C19H40	007225-66-3	87
3	2-Bromotetradecane	276	C14H29Br	074036-95-6	83
4	Pentacosane	352	C25H52	000629-99-2	83
5	Heneicosane	296	C21H44	000629-94-7	81

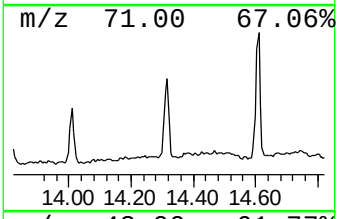


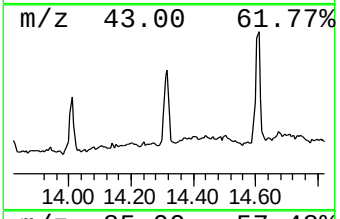


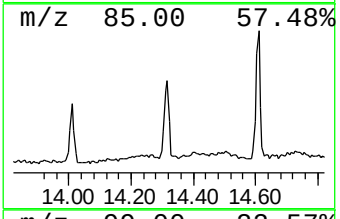


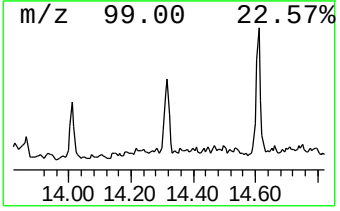












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Data File : BF113553.D
Acq On : 3 Apr 2019 19:47
Operator : JU/SJ
Sample : K2213-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S9C(2-10)COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

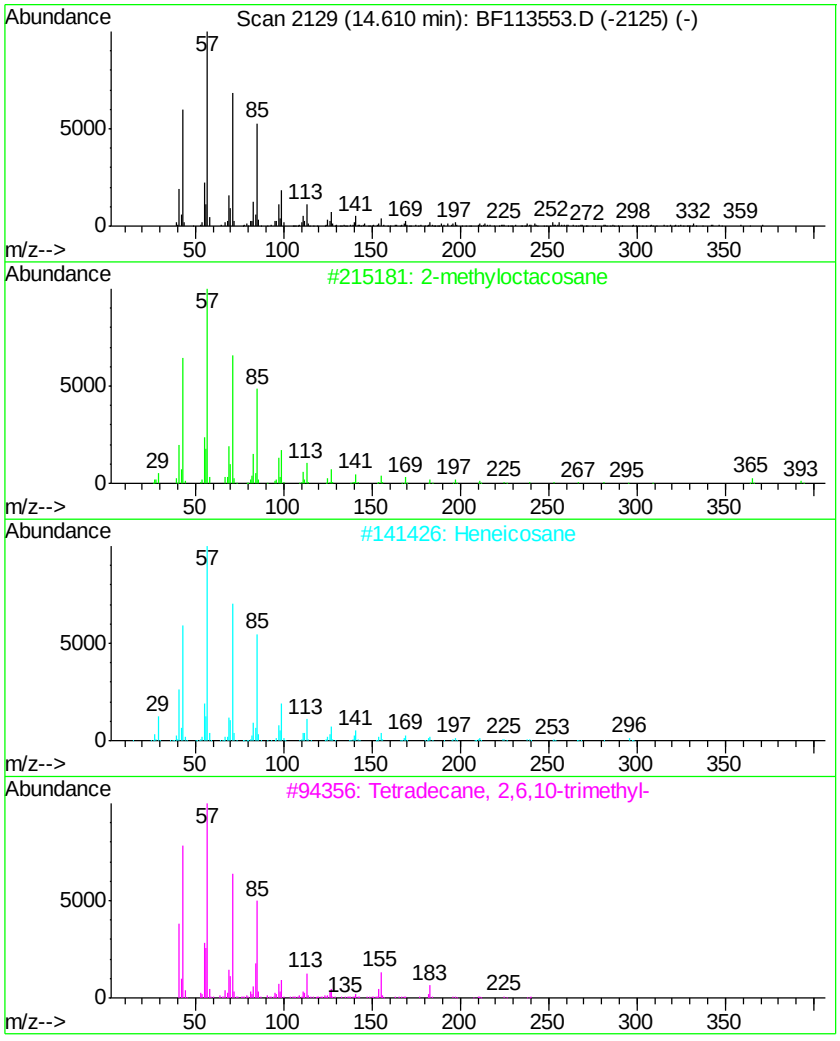
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

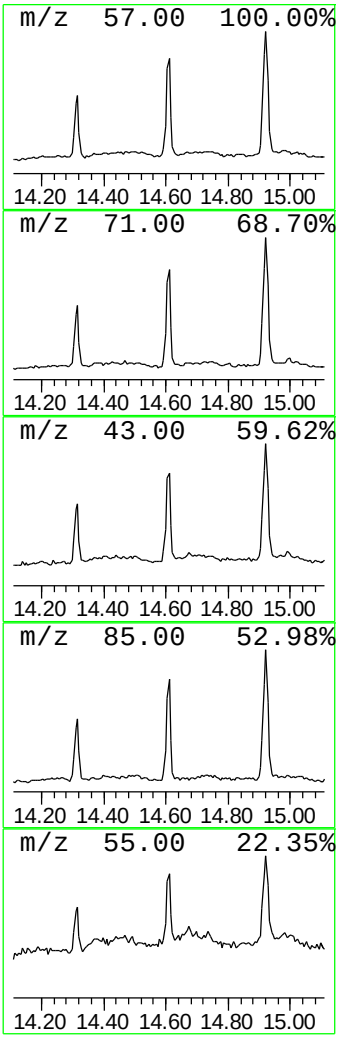
****

Peak Number 7 2-methyloctacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.61	3.52 ng	229989	Perylene-d12	15.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	90
2	Heneicosane	296	C21H44	000629-94-7	90
3	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	90
4	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	86
5	Hexatriacontane	507	C36H74	000630-06-8	86





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040319\
Data File : BF113553.D
Acq On : 3 Apr 2019 19:47
Operator : JU/SJ
Sample : K2213-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S9C(2-10)COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.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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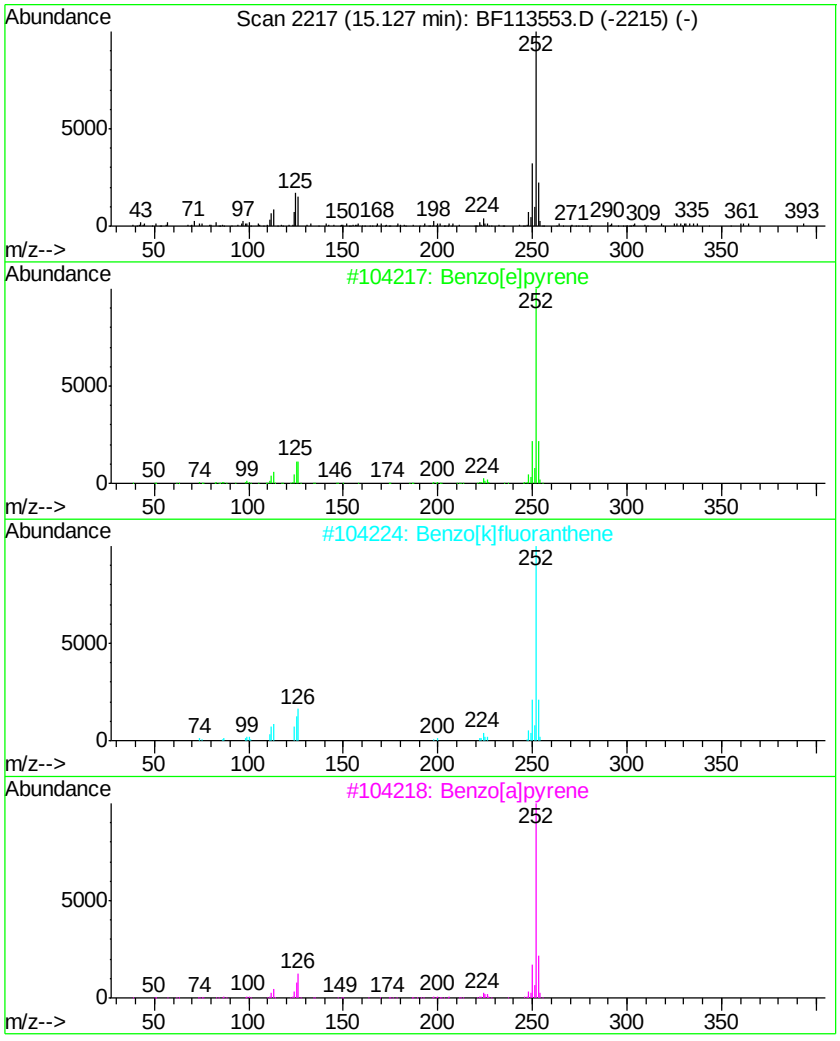
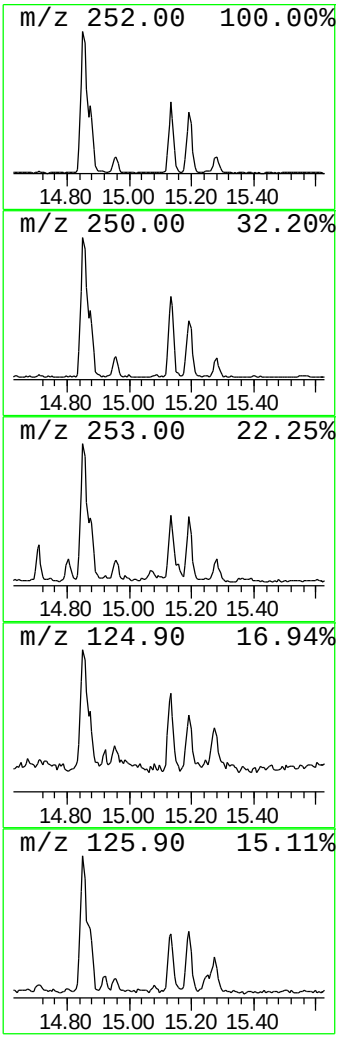
Peak Number 8 Benzo[e]pyrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.13	2.38 ng	155120	Perylene-d12	15.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
3	Benzo[a]pyrene	252	C20H12	000050-32-8	96
4	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	94
5	Perylene	252	C20H12	000198-55-0	93





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Acq On : 3 Apr 2019 19:47
Operator : JU/SJ
Sample : K2213-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S9C(2-10)COMP

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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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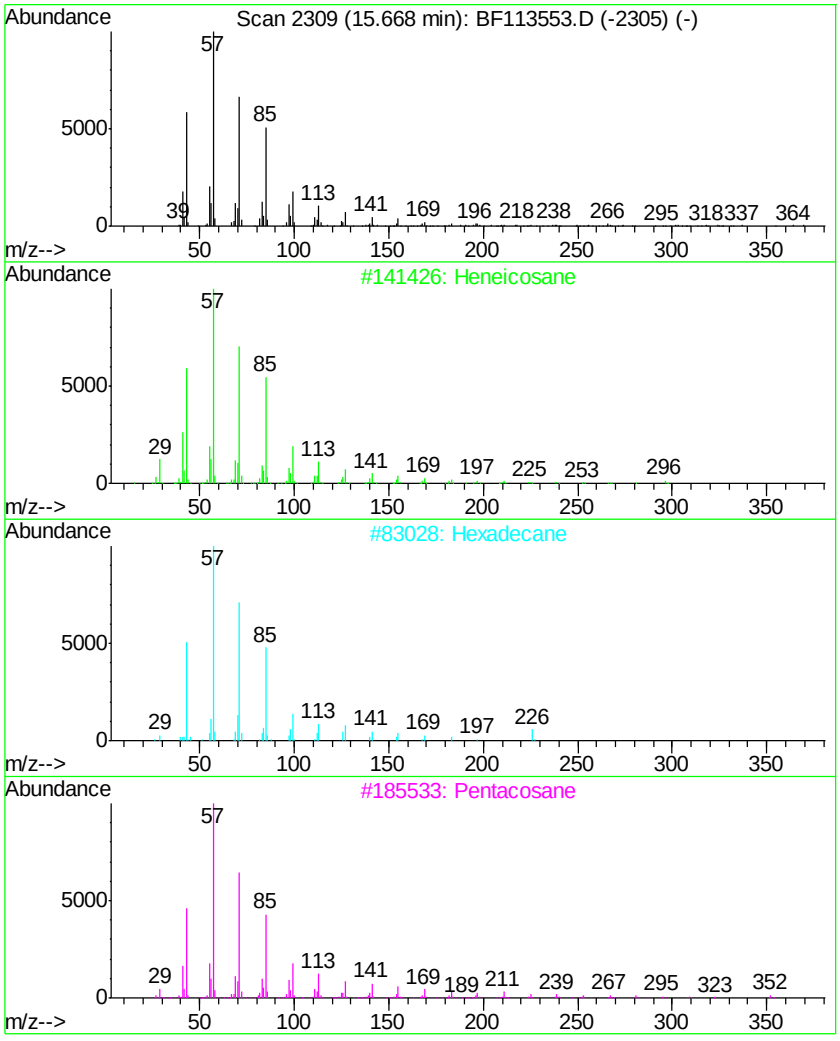
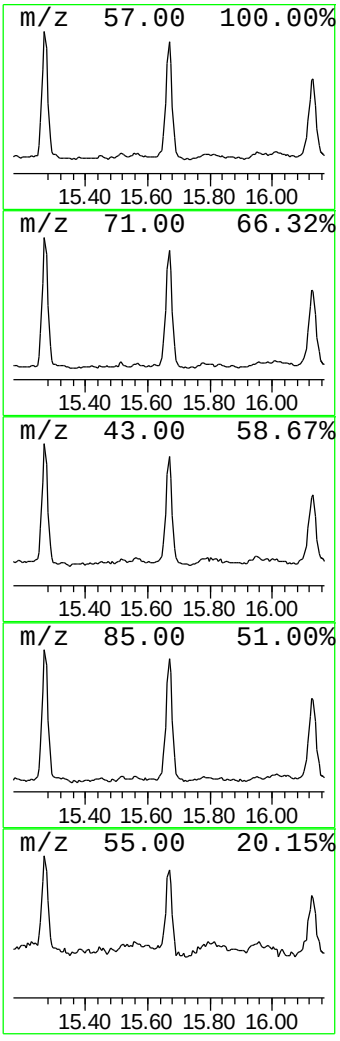
Peak Number 9 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.67	6.56 ng	428204	Perylene-d12	15.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hexadecane	226	C16H34	000544-76-3	87
3	Pentacosane	352	C25H52	000629-99-2	86
4	Nonadecane	268	C19H40	000629-92-5	83
5	Hexacosane	366	C26H54	000630-01-3	81





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Acq On : 3 Apr 2019 19:47
Operator : JU/SJ
Sample : K2213-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S9C(2-10)COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.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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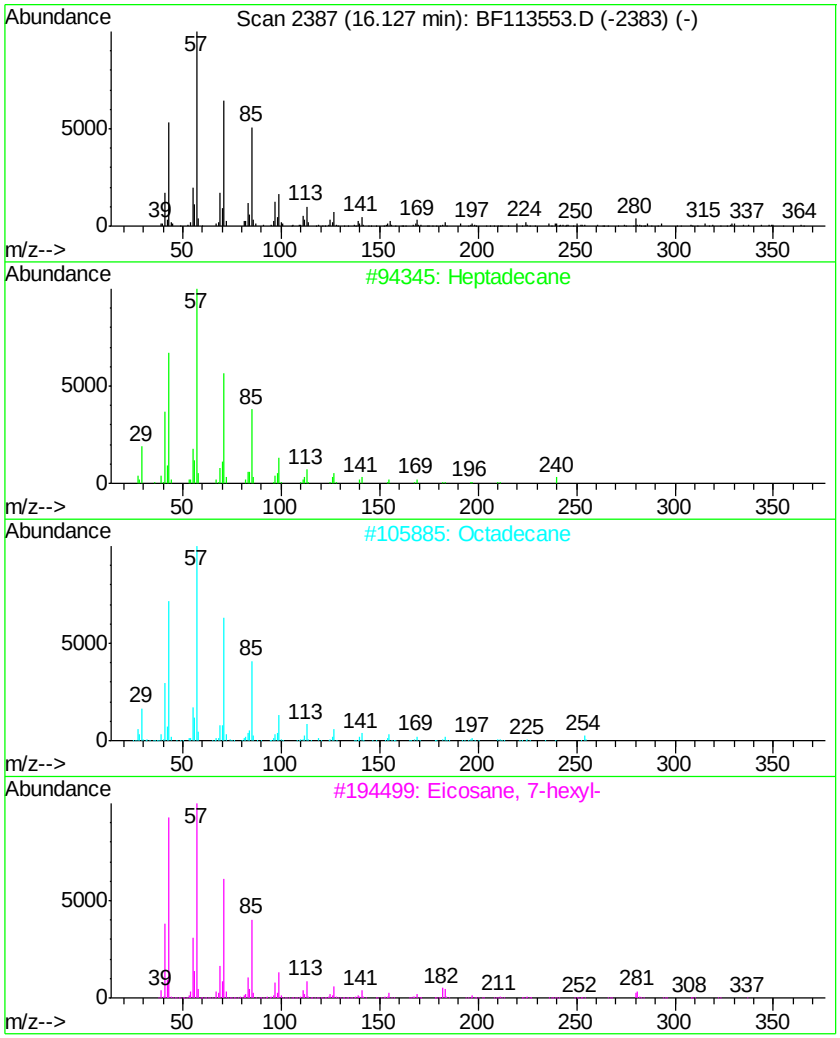
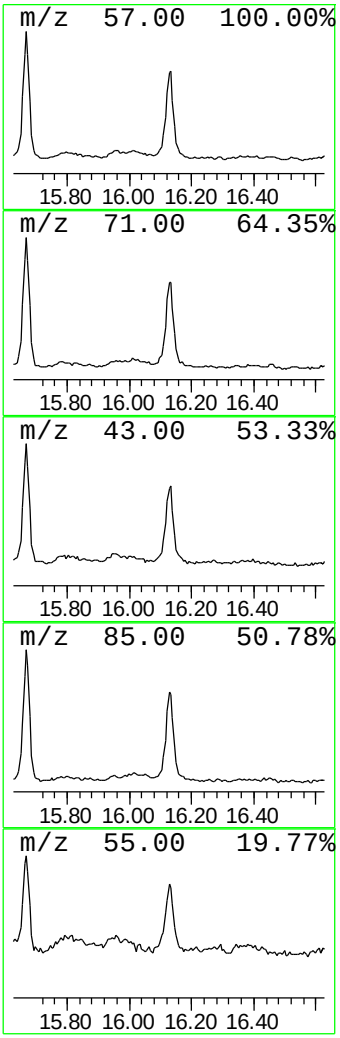
Peak Number 10 Heptadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	6.41 ng	418146	Perylene-d12	15.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Octadecane	254	C18H38	000593-45-3	91
3	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
4	Heneicosane	296	C21H44	000629-94-7	90
5	Tetracosane	338	C24H50	000646-31-1	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040319\
Data File : BF113553.D
Acq On : 3 Apr 2019 19:47
Operator : JU/SJ
Sample : K2213-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S9C(2-10)COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.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
unknown6.46	6.46	91.1	ng	3520910	1	6.69	773035	20.0
n-Hexadecanoic acid	11.74	5.5	ng	231800	4	11.20	848729	20.0
Octadecanoic acid	12.53	4.8	ng	278529	5	13.84	1165030	20.0
1-Octadecene	13.72	10.4	ng	603100	5	13.84	1165030	20.0
Octadecane	14.32	2.3	ng	132068	5	13.84	1165030	20.0
2-methyloctacosane	14.61	3.5	ng	229989	6	15.25	1304940	20.0
Benzo[e]pyrene	15.13	2.4	ng	155120	6	15.25	1304940	20.0
Heneicosane	15.67	6.6	ng	428204	6	15.25	1304940	20.0
Heptadecane	16.13	6.4	ng	418146	6	15.25	1304940	20.0