LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031319\
Data File : BF113045.D
Acq On : 13 Mar 2019 23:11
Operator : JU/SJ
Sample : K1870-05 5X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-2

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-BF022719.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF113044.D

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.334	548	552	565	rBV	746210	699772	37.42%	3.690%
2	6.363	723	727	743	rBV	866367	777247	41.57%	4.099%
3	6.492	746	749	759	rBV	897216	790094	42.25%	4.167%
4	6.728	785	789	792	rBV	1109465	966653	51.69%	5.098%
5	6.881	811	815	824	rBV	774351	615653	32.92%	3.247%
6	7.281	880	883	896	rBV	500631	460262	24.61%	2.427%
7	7.916	987	991	995	rBV	37964	35732	1.91%	0.188%
8	8.010	1003	1007	1013	rBV	1454462	1342072	71.77%	7.077%
9	9.081	1186	1189	1203	rBV	1050523	936213	50.07%	4.937%
10	9.475	1253	1256	1265	rVB	73493	64640	3.46%	0.341%
11	9.757	1300	1304	1308	rBV2	1871884	1646704	88.06%	8.684%
12	9.786	1308	1309	1318	rVB	44225	42190	2.26%	0.222%
13	10.275	1389	1392	1394	rVB2	23958	19185	1.03%	0.101%
14	10.304	1394	1397	1400	rBV	20202	20771	1.11%	0.110%
15	10.539	1433	1437	1449	rBV	824250	735969	39.36%	3.881%
16	11.098	1526	1532	1533	rBV4	13667	22528	1.20%	0.119%
17	11.233	1552	1555	1558	rBV	1789362	1781282	95.26%	9.394%
18	11.257	1558	1559	1565	rVV	402281	281482	15.05%	1.484%
19	11.310	1565	1568	1573	rVB	89623	80309	4.29%	0.424%
20	11.469	1592	1595	1601	rBV	15679	24275	1.30%	0.128%
21	11.698	1631	1634	1637	rBV5	15167	20228	1.08%	0.107%
22	11.733	1637	1640	1643	rVV	55208	64900	3.47%	0.342%
23	11.769	1643	1646	1651	rVV2	244161	304202	16.27%	1.604%
24	11.810	1651	1653	1656	rVV	46210	55403	2.96%	0.292%
25	11.845	1656	1659	1662	rVV	92234	116173	6.21%	0.613%
26	11.869	1662	1663	1668	rVB	46261	33438	1.79%	0.176%
27	12.027	1687	1690	1692	rBV	35327	34896	1.87%	0.184%
28	12.280	1731	1733	1736	rBV	36346	39829	2.13%	0.210%
29	12.363	1745	1747	1752	rVB5	23041	29018	1.55%	0.153%
30	12.439	1757	1760	1764	rBV	566994	499239	26.70%	2.633%
31	12.557	1777	1780	1783	rBV4	40110	45629	2.44%	0.241%
32	12.669	1793	1799	1802	rBV	470087	507617	27.15%	2.677%
33	12.739	1809	1811	1816	rVB	80211	73936	3.95%	0.390%
34	12.810	1820	1823	1830	rVB	990590	961748	51.43%	5.072%

LSC Area Percent Report

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Acq On : 13 Mar 2019 23:11
Operator : JU/SJ
Sample : K1870-05 5X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-2

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-BF022719.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.998	1852	1855	1858	rVB	61606	57170	3.06%	0.301%
36	13.063	1863	1866	1869	rVB2	61025	52464	2.81%	0.277%
37	13.098	1870	1872	1875	rVB	32691	31823	1.70%	0.168%
38	13.221	1890	1893	1898	rBV2	32716	35736	1.91%	0.188%
39	13.663	1966	1968	1974	rBV4	33399	39299	2.10%	0.207%
40	13.716	1974	1977	1983	rBV2	156907	194601	10.41%	1.026%
41	13.863	1996	2002	2005	rBV	1663016	1869951	100.00%	9.861%
42	13.886	2005	2006	2011	rVB	232084	147200	7.87%	0.776%
43	14.345	2081	2084	2086	rBV2	93876	100982	5.40%	0.533%
44	14.868	2170	2173	2176	rBV	179427	238430	12.75%	1.257%
45	14.951	2184	2187	2196	rVB2	201032	275768	14.75%	1.454%
46	15.145	2218	2220	2226	rVB	104381	121288	6.49%	0.640%
47	15.204	2228	2230	2234	rVB	114981	119288	6.38%	0.629%
48	15.268	2236	2241	2245	rBV	945241	1128229	60.33%	5.950%
49	15.710	2312	2316	2321	rBV	294872	421401	22.54%	2.222%

Sum of corrected areas: 18962919

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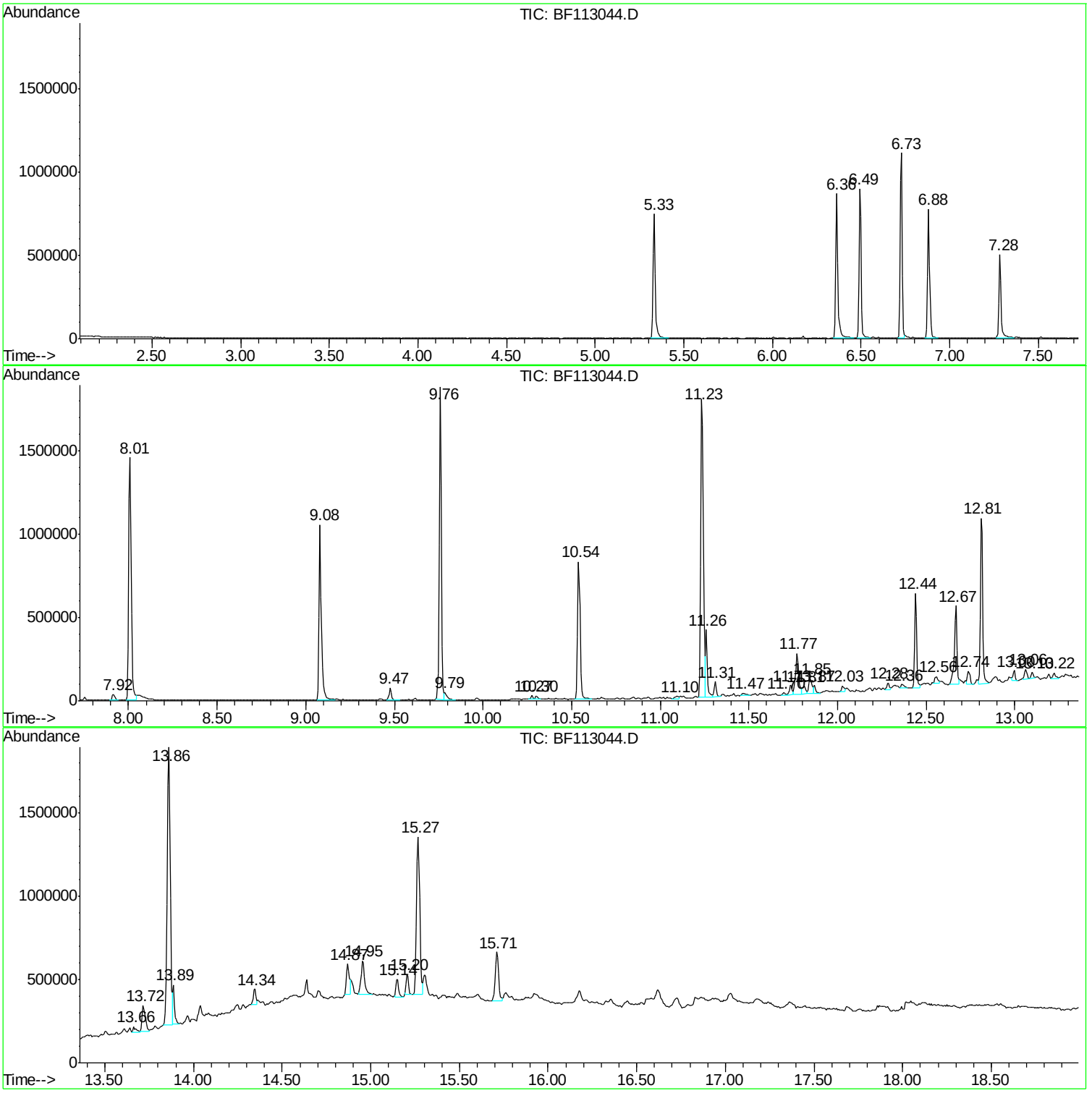
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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\BF031319\
Data File : BF113045.D
Acq On : 13 Mar 2019 23:11
Operator : JU/SJ
Sample : K1870-05 5X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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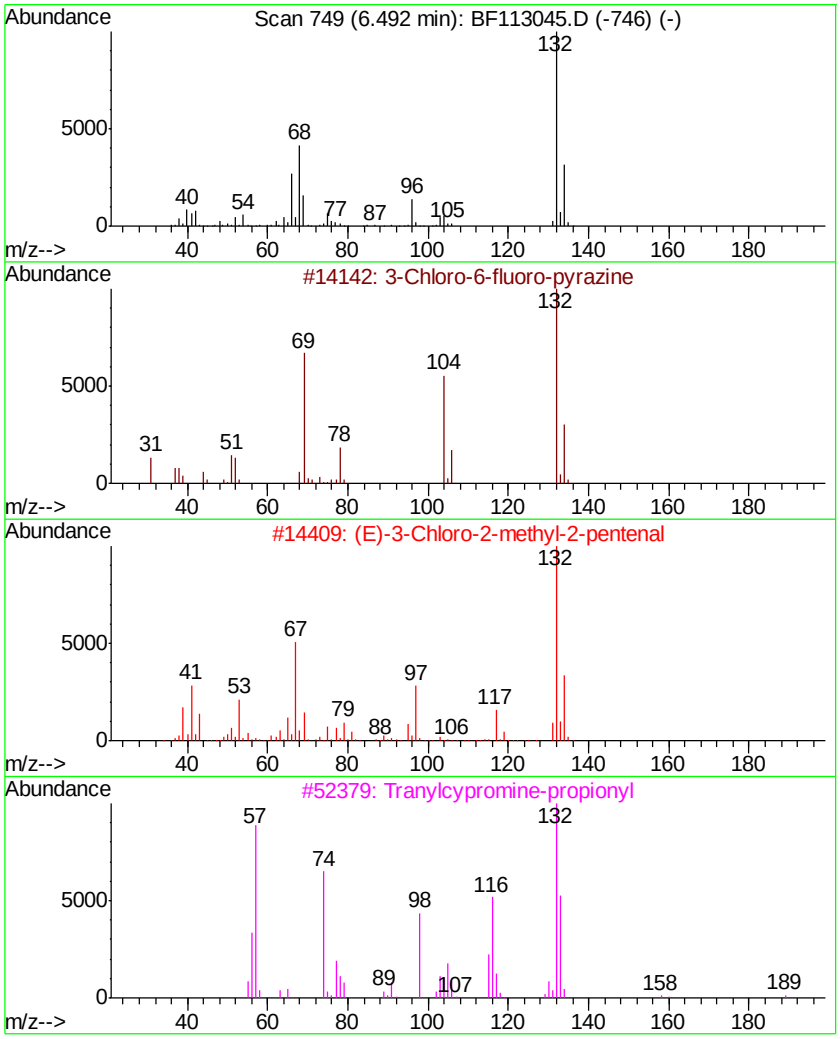
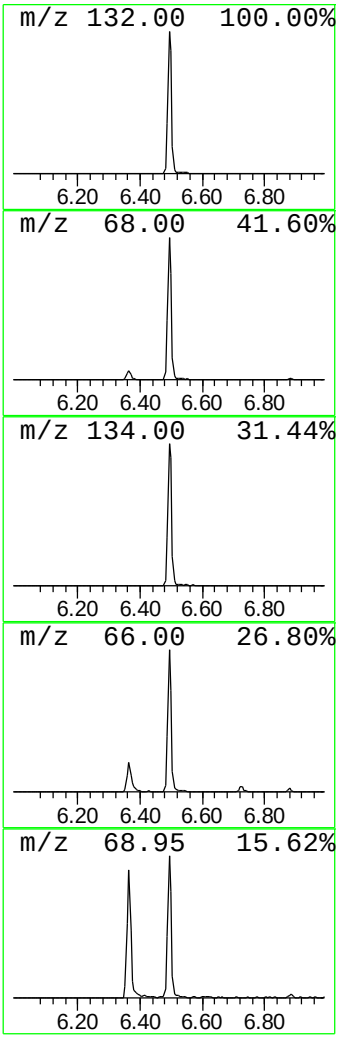
Peak Number 1 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	16.35 ng	790094	1,4-Dichlorobenzene-d4	6.73

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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031319\
Data File : BF113045.D
Acq On : 13 Mar 2019 23:11
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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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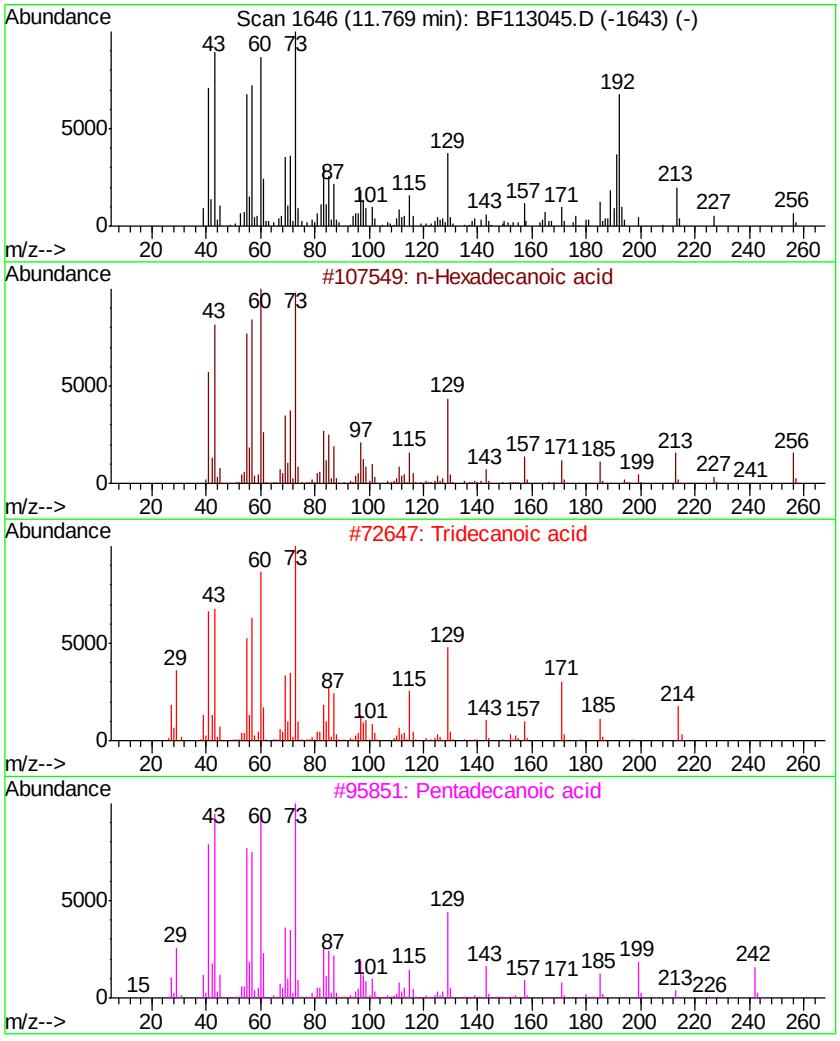
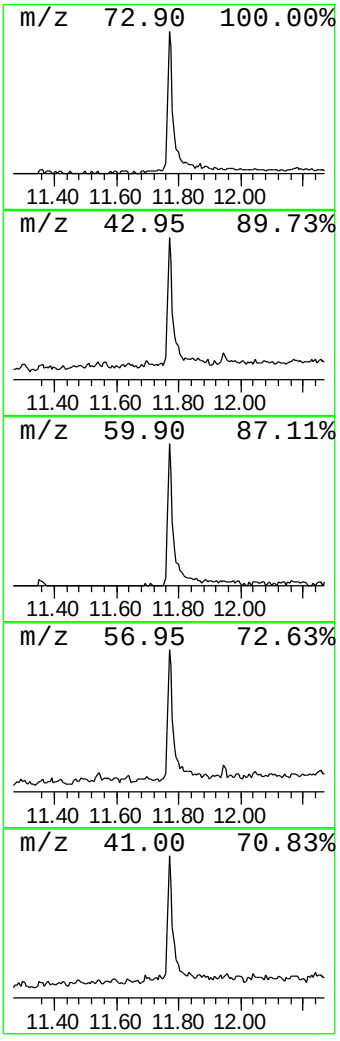
Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	3.42 ng	304202	Phenanthrene-d10	11.23

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	86
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	52
5	n-Decanoic acid	172	C10H20O2	000334-48-5	41





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031319\
Data File : BF113045.D
Acq On : 13 Mar 2019 23:11
Operator : JU/SJ
Sample : K1870-05 5X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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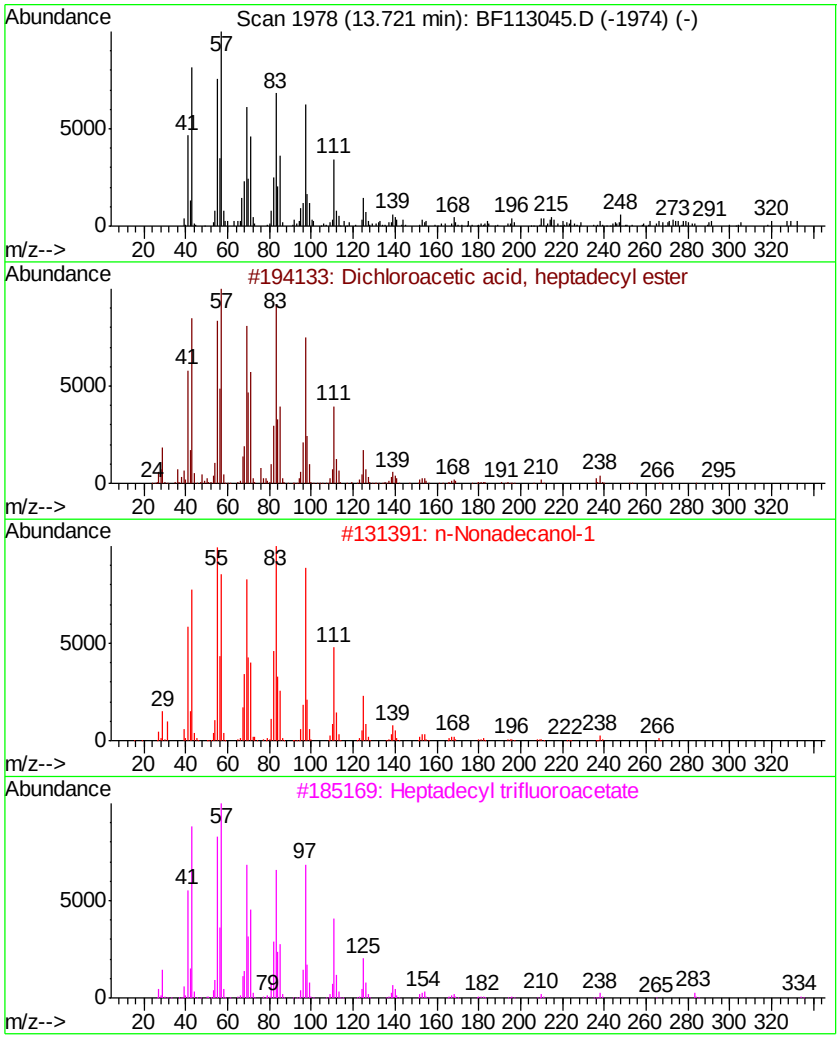
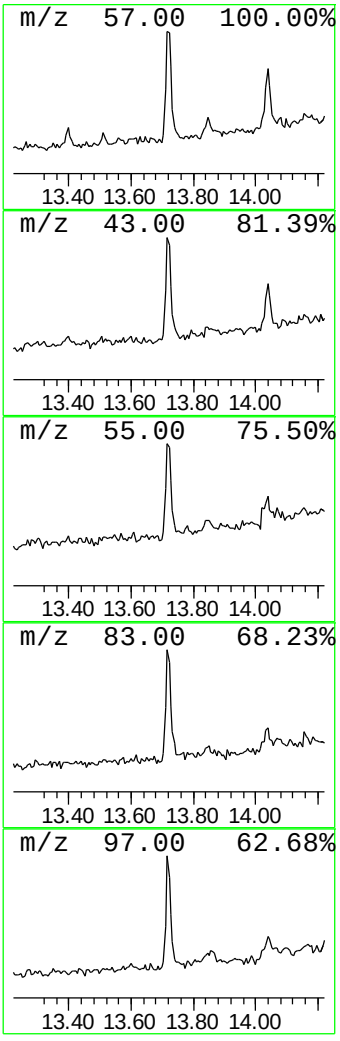
Peak Number 4 Dichloroacetic acid, heptad... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	2.08 ng	194601	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
4	Behenic alcohol	326	C22H46O	000661-19-8	93
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031319\
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Sample : K1870-05 5X
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Instrument : BNA_F
ClientSampleId : SP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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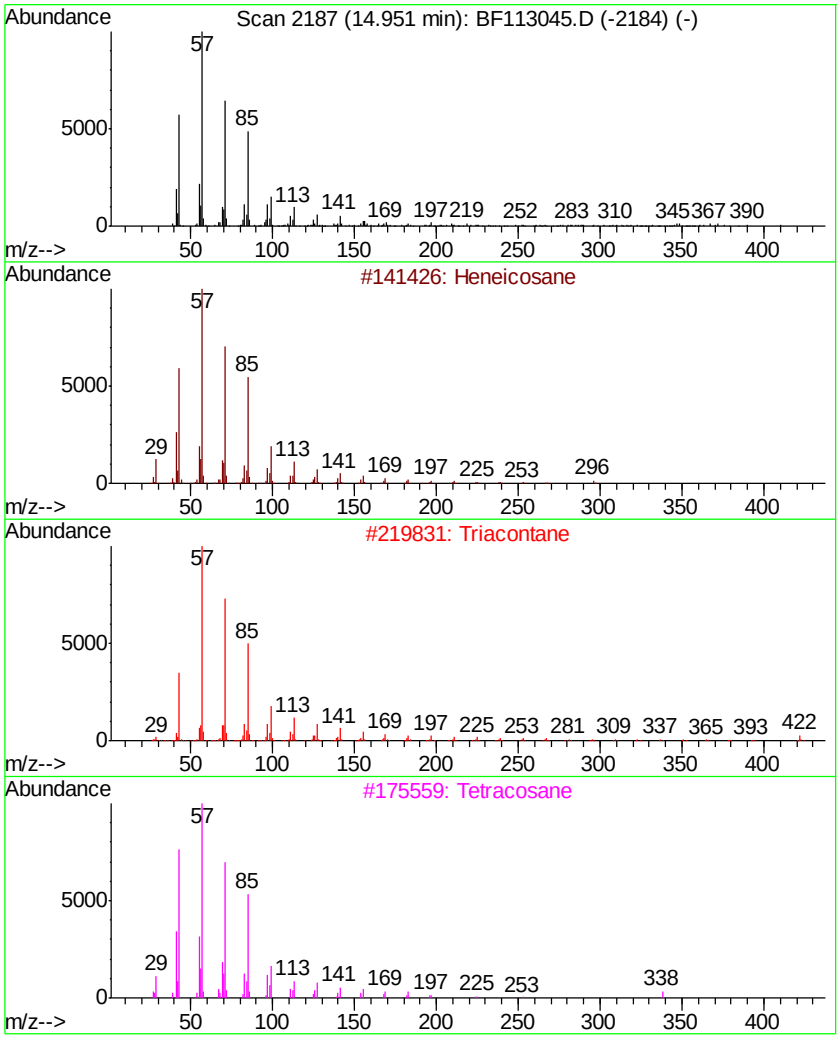
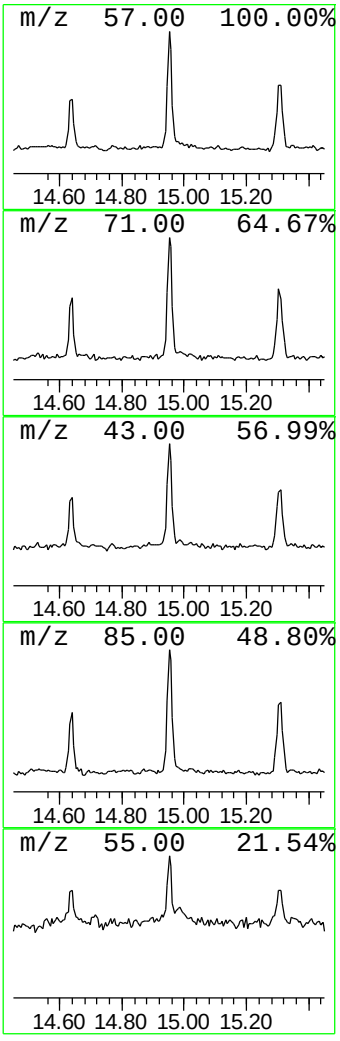
Peak Number 5 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	4.89 ng	275768	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Triacontane	422	C30H62	000638-68-6	87
3	Tetracosane	338	C24H50	000646-31-1	87
4	Nonadecane	268	C19H40	000629-92-5	86
5	2-methyloctacosane	408	C29H60	1000376-72-8	86





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Misc :
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Instrument : BNA_F
ClientSampleId : SP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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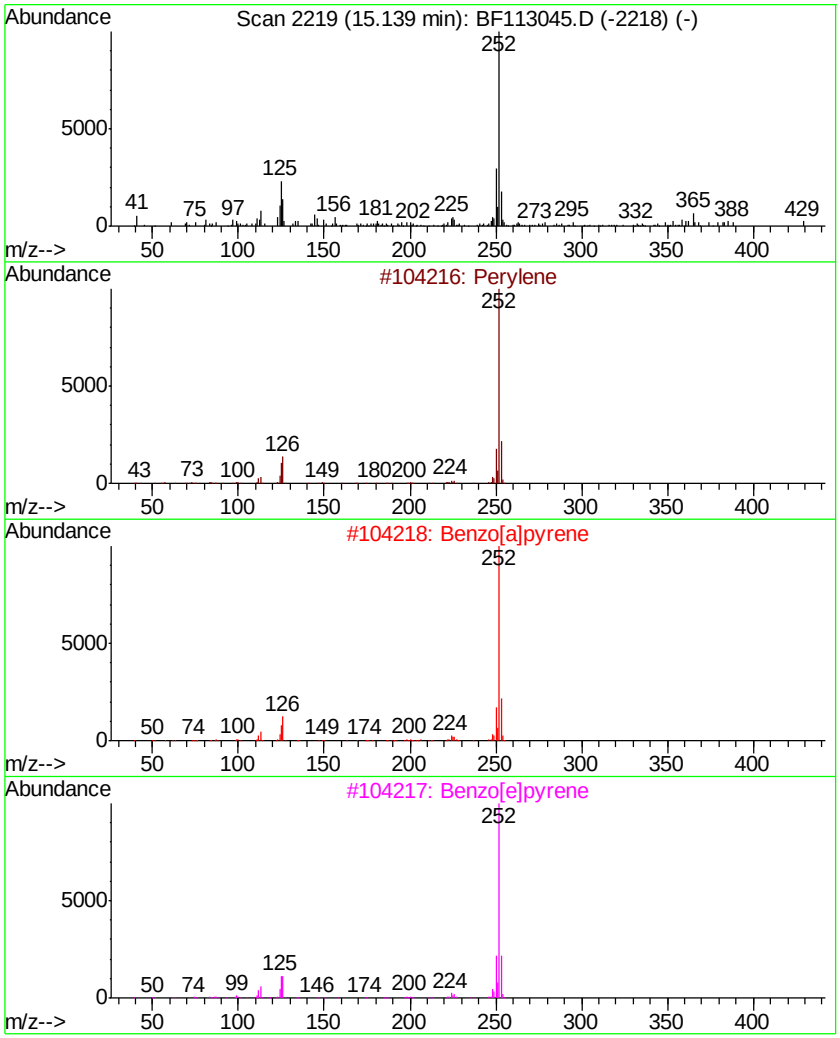
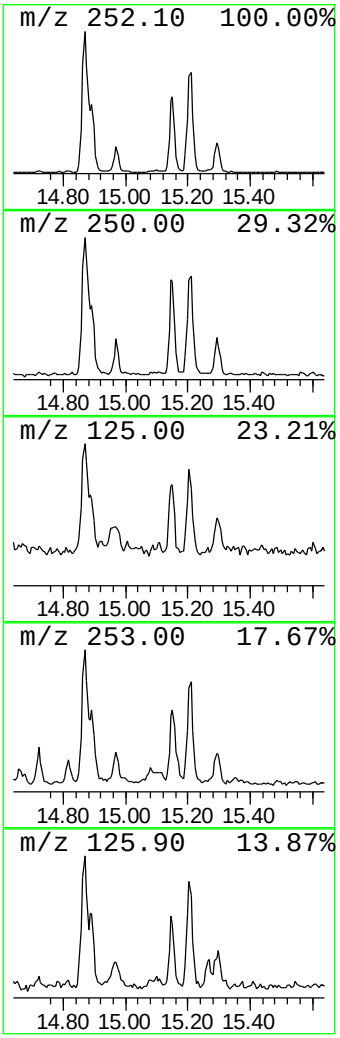
Peak Number 6 Perylene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.14	2.15 ng	121288	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	96
2	Benzo[a]pyrene	252	C20H12	000050-32-8	95
3	Benzo[e]pyrene	252	C20H12	000192-97-2	91
4	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	91
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	89





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Sample : K1870-05 5X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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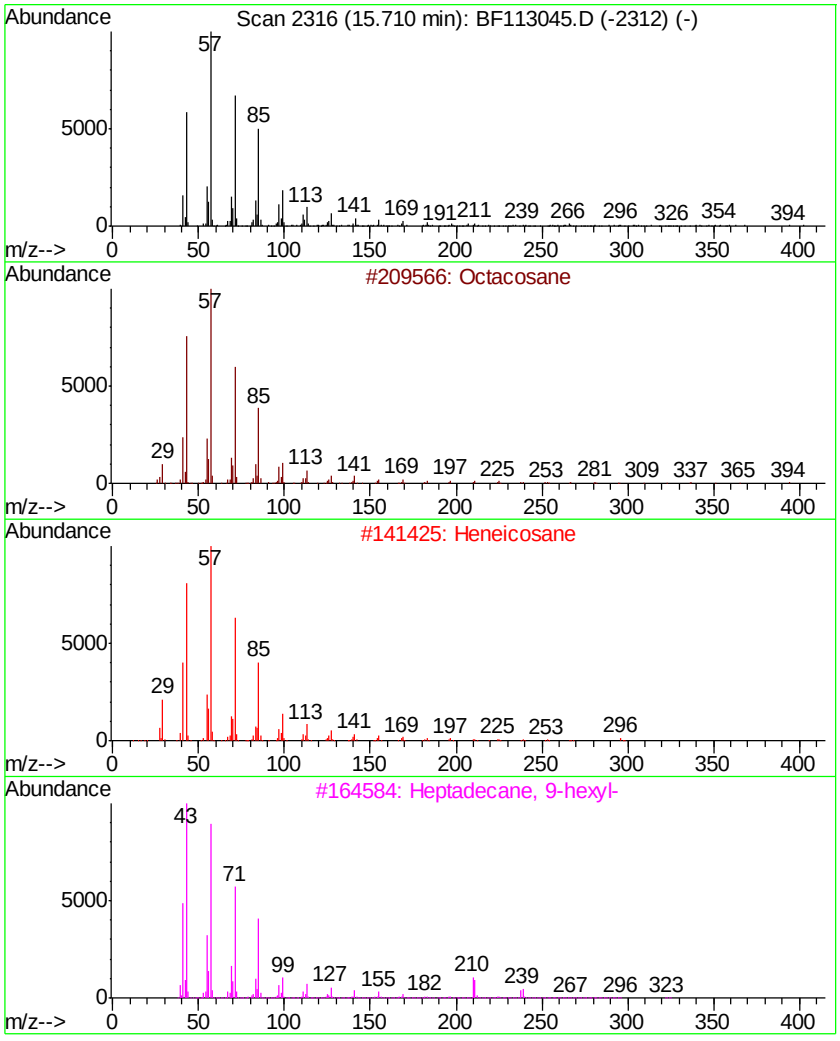
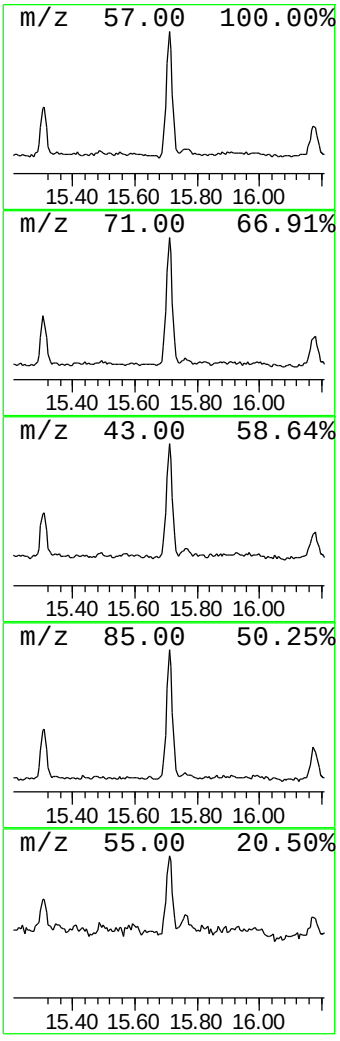
Peak Number 7 Octacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	7.47 ng	421401	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	98
2	Heneicosane	296	C21H44	000629-94-7	95
3	Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	94
4	Hexacosane	366	C26H54	000630-01-3	91
5	Tetratetracontane	619	C44H90	007098-22-8	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031319\
Data File : BF113045.D
Acq On : 13 Mar 2019 23:11
Operator : JU/SJ
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Misc :
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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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
unknown6.49	6.49	16.4	ng	790094	1	6.73	966653	20.0
n-Hexadecanoic acid	11.77	3.4	ng	304202	4	11.23	1781280	20.0
Dichloroacetic ac...	13.72	2.1	ng	194601	5	13.86	1869950	20.0
Heneicosane	14.95	4.9	ng	275768	6	15.27	1128230	20.0
Perylene	15.14	2.1	ng	121288	6	15.27	1128230	20.0
Octacosane	15.71	7.5	ng	421401	6	15.27	1128230	20.0