LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090319\
Data File : BF116781.D
Acq On : 3 Sep 2019 19:12
Operator : HP/JU
Sample : K4554-41
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3-(0-2)

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-BF083019.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	5.463	569	574	578	rBV	2659318	2656278	86.84%	8.846%
2	6.481	741	747	749	rBV	2742461	2827076	92.42%	9.415%
3	6.616	766	770	773	rBV	3172089	2888609	94.43%	9.620%
4	6.845	806	809	813	rBV	948159	761147	24.88%	2.535%
5	7.004	832	836	839	rBV	2687280	2186663	71.49%	7.282%
6	7.404	899	904	907	rBV	1999734	1778977	58.16%	5.924%
7	8.128	1023	1027	1030	rBV	1288095	1004712	32.85%	3.346%
8	9.204	1206	1210	1213	rBV	3623098	3058890	100.00%	10.187%
9	9.286	1220	1224	1228	rBV3	24449	34629	1.13%	0.115%
10	9.539	1264	1267	1270	rBV	40184	38521	1.26%	0.128%
11	9.592	1273	1276	1285	rVB	243964	217996	7.13%	0.726%
12	9.880	1321	1325	1328	rBV	1428274	1138772	37.23%	3.792%
13	9.922	1328	1332	1339	rVB4	17099	35187	1.15%	0.117%
14	10.180	1371	1376	1377	rBV2	56605	84321	2.76%	0.281%
15	10.286	1391	1394	1397	rBV3	44055	44951	1.47%	0.150%
16	10.669	1454	1459	1462	rBV	1978998	1892172	61.86%	6.301%
17	10.798	1476	1481	1485	rBV2	56358	84066	2.75%	0.280%
18	11.363	1573	1577	1579	rBV	1349413	1110038	36.29%	3.697%
19	11.386	1579	1581	1584	rVV	163580	135344	4.42%	0.451%
20	11.433	1587	1589	1592	rVB	39506	36591	1.20%	0.122%
21	11.657	1625	1627	1632	rBV	40481	35301	1.15%	0.118%
22	11.863	1656	1662	1663	rBV2	39954	45305	1.48%	0.151%
23	11.886	1663	1666	1671	rVV	342053	307255	10.04%	1.023%
24	11.969	1678	1680	1683	rBV2	45372	44256	1.45%	0.147%
25	12.063	1694	1696	1699	rVB	48436	39632	1.30%	0.132%
26	12.451	1759	1762	1764	rBV2	68667	59302	1.94%	0.197%
27	12.574	1779	1783	1786	rBV	284509	231675	7.57%	0.772%
28	12.669	1796	1799	1802	rBV4	75444	77936	2.55%	0.260%
29	12.798	1816	1821	1823	rBV	247404	216322	7.07%	0.720%
30	12.821	1823	1825	1828	rVB2	53790	42300	1.38%	0.141%
31	12.945	1842	1846	1849	rBV	2748453	2526519	82.60%	8.414%
32	13.174	1883	1885	1891	rBV2	56427	68890	2.25%	0.229%
33	13.516	1941	1943	1950	rVB	71710	64077	2.09%	0.213%
34	13.633	1960	1963	1974	rVB2	66605	91758	3.00%	0.306%

LSC Area Percent Report

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Sample : K4554-41
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3-(0-2)

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-BF083019.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.833	1994	1997	2006	rVB2	306245	429995	14.06%	1.432%
36	13.992	2019	2024	2027	rBV	981434	967580	31.63%	3.222%
37	14.016	2027	2028	2031	rVB	99844	55897	1.83%	0.186%
38	14.163	2049	2053	2058	rVB	125814	132577	4.33%	0.442%
39	14.468	2102	2105	2109	rBV2	199955	212145	6.94%	0.706%
40	14.768	2153	2156	2159	rBV	188505	182286	5.96%	0.607%
41	15.021	2196	2199	2203	rBV	92988	141988	4.64%	0.473%
42	15.104	2209	2213	2216	rBV	231522	256639	8.39%	0.855%
43	15.321	2248	2250	2257	rVB	62347	70698	2.31%	0.235%
44	15.380	2257	2260	2264	rVV	85236	107475	3.51%	0.358%
45	15.451	2267	2272	2275	rVV	704804	925625	30.26%	3.082%
46	15.480	2275	2277	2283	rVB	202129	224213	7.33%	0.747%
47	15.910	2346	2350	2355	rBV	195869	265005	8.66%	0.883%
48	16.409	2431	2435	2445	rVB2	107026	190832	6.24%	0.636%

Sum of corrected areas: 30028423

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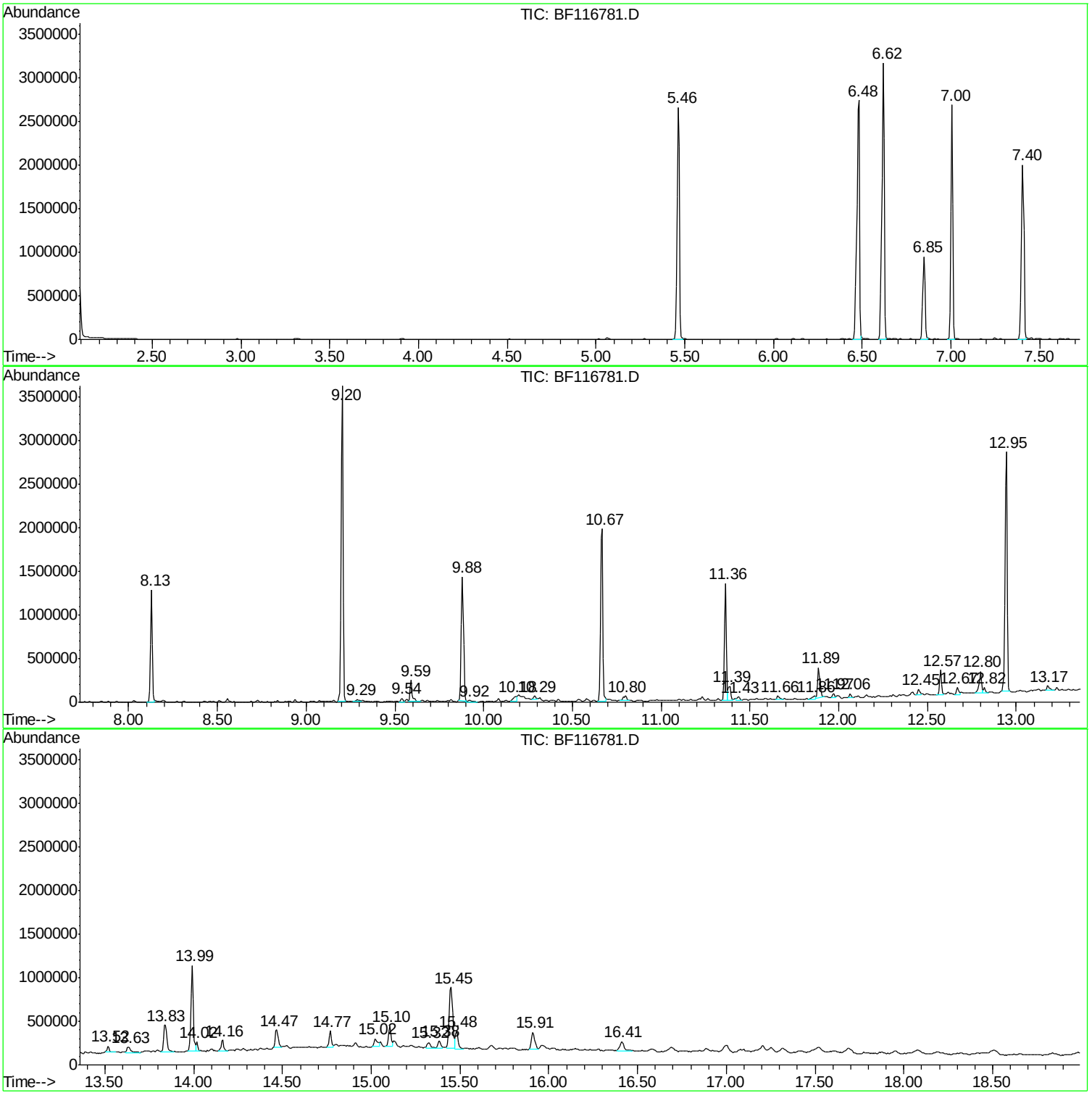
Instrument :
BNA_F
ClientSampleId :
SB-3-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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

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Data File : BF116781.D
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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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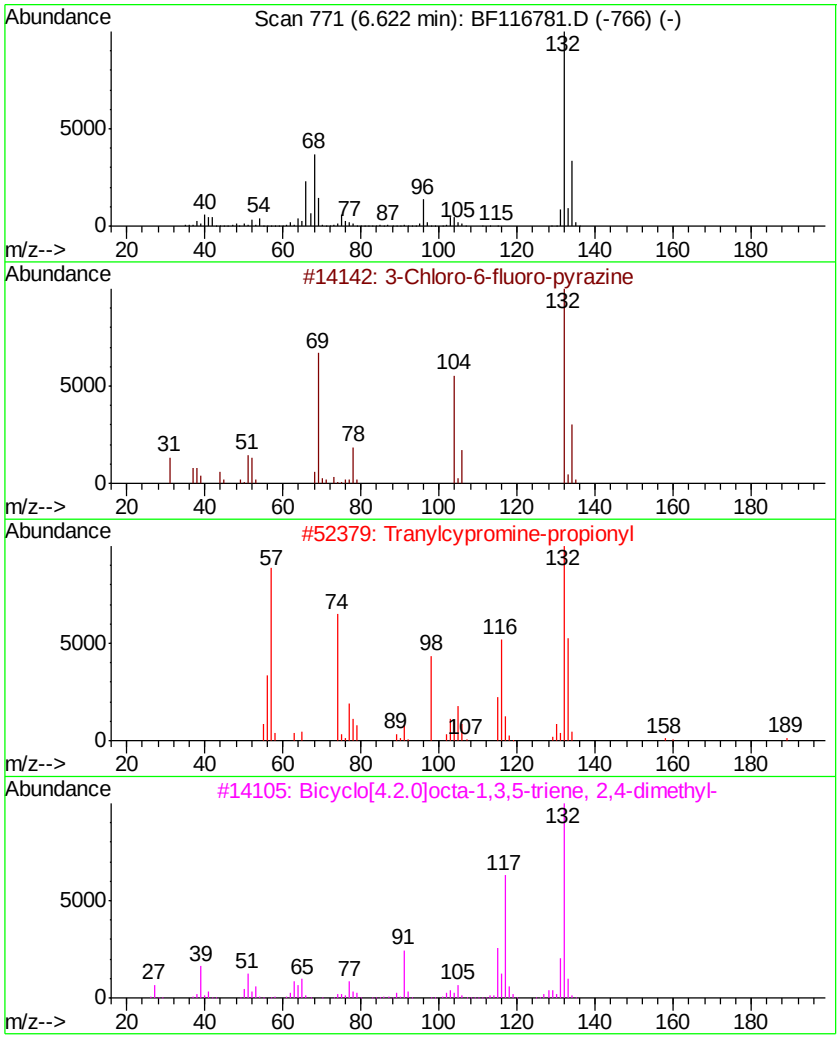
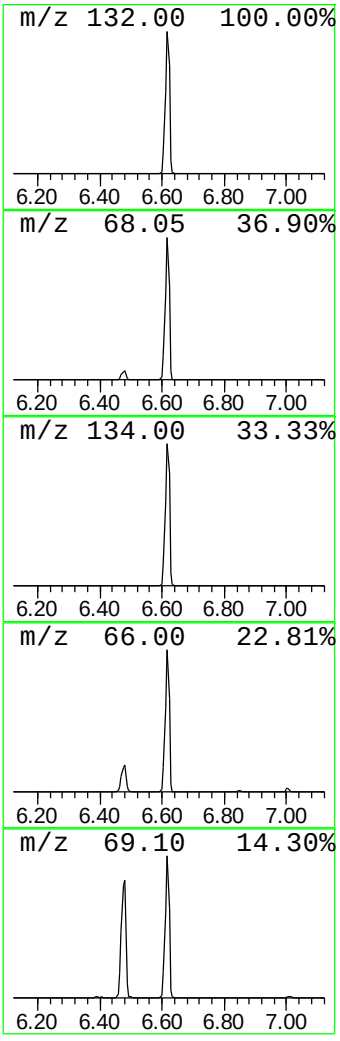
Peak Number 1 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	75.90 ng	2888610	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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Instrument : BNA_F
ClientSampleId : SB-3-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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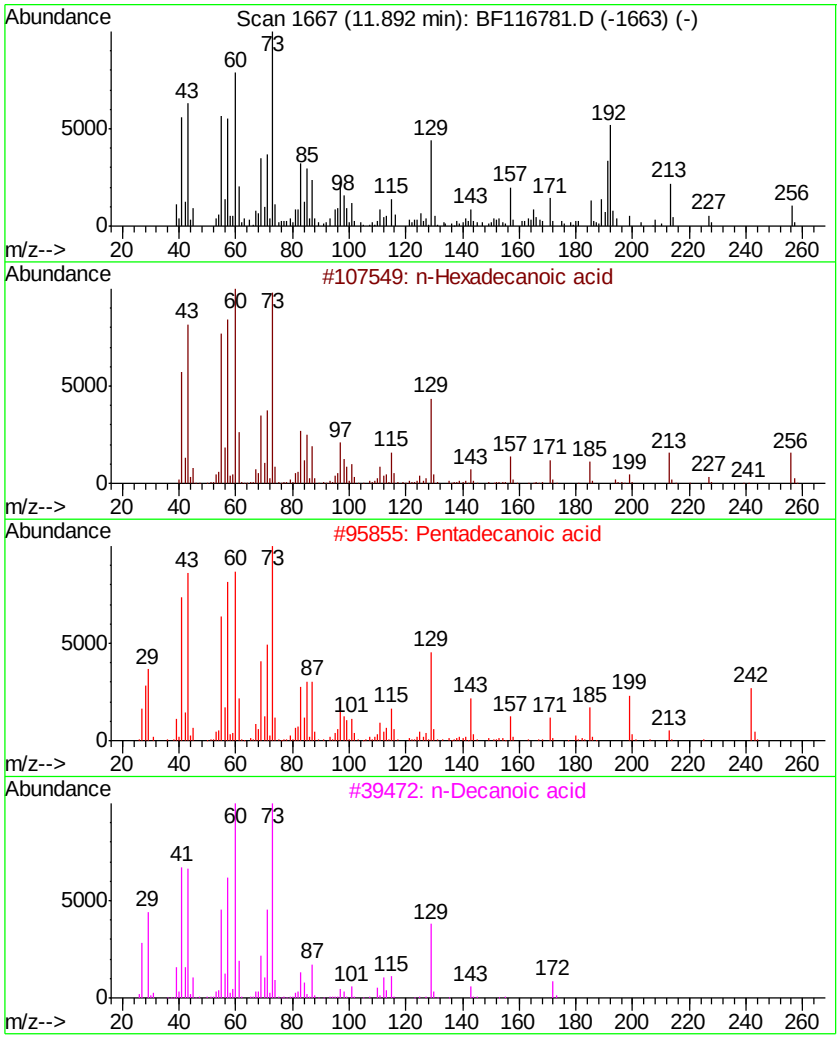
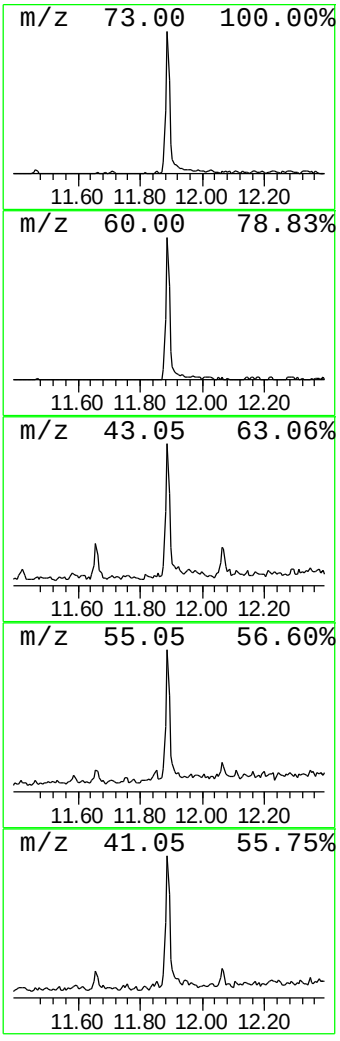
Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.89	5.54 ng	307255	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	n-Decanoic acid	172	C10H20O2	000334-48-5	76
4	Tridecanoic acid	214	C13H26O2	000638-53-9	68
5	Octane, 2-methyl-	128	C9H20	003221-61-2	25





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090319\
Data File : BF116781.D
Acq On : 3 Sep 2019 19:12
Operator : HP/JU
Sample : K4554-41
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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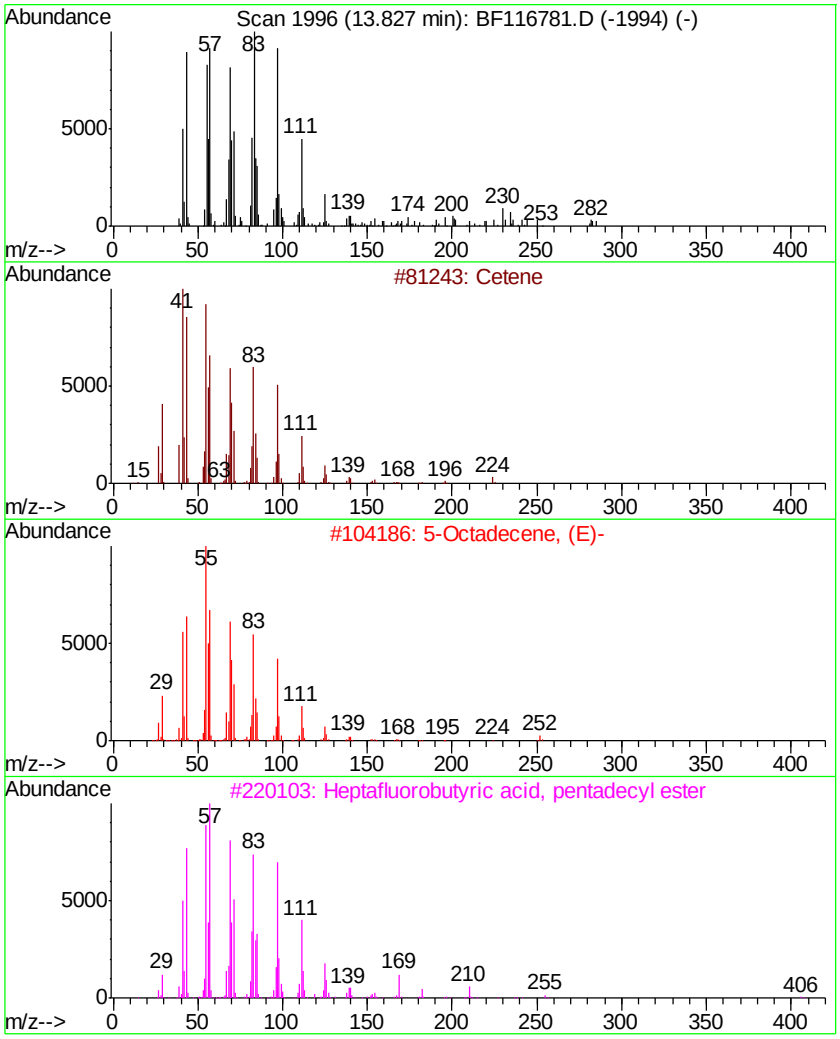
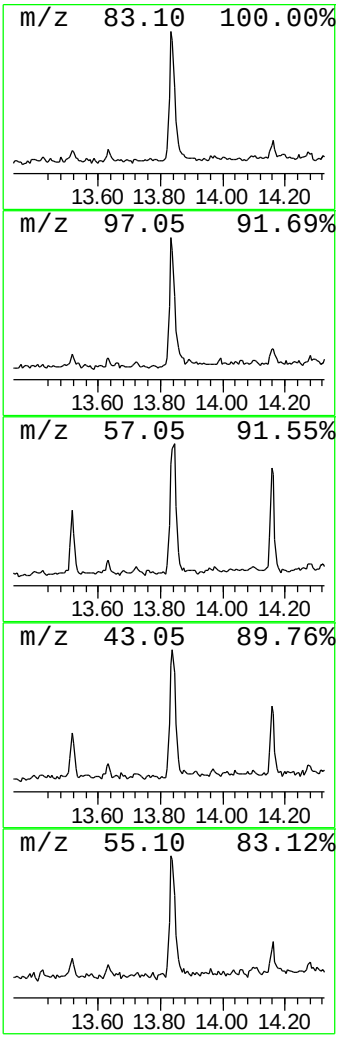
Peak Number 4 Cetene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	8.89 ng	429995	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cetene	224	C16H32	000629-73-2	96
2	5-Octadecene, (E)-	252	C18H36	007206-21-5	95
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : SB-3-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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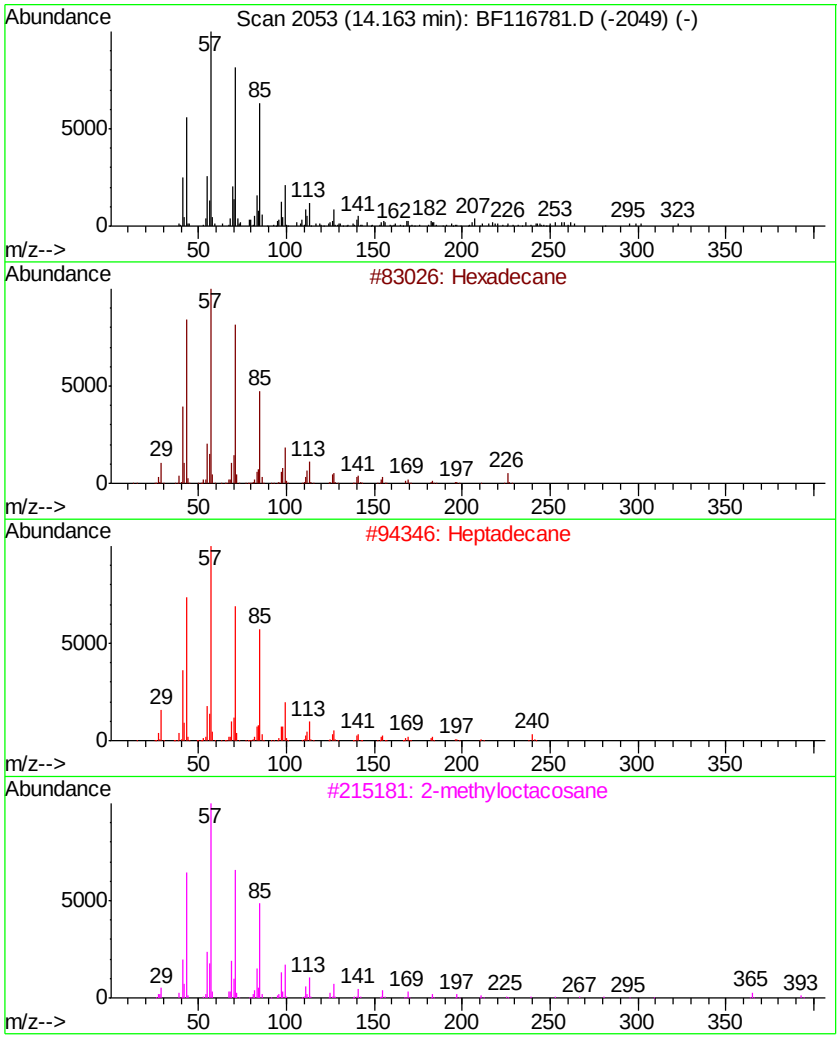
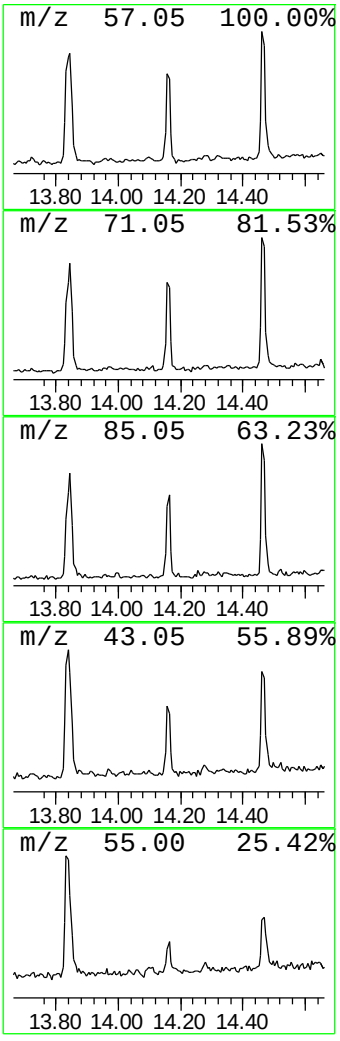
Peak Number 5 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.16	2.74 ng	132577	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	94
2	Heptadecane	240	C17H36	000629-78-7	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Hexacosane	366	C26H54	000630-01-3	90
5	Dodecane, 2-methyl-	184	C13H28	001560-97-0	90





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Instrument : BNA_F
ClientSampleId : SB-3-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
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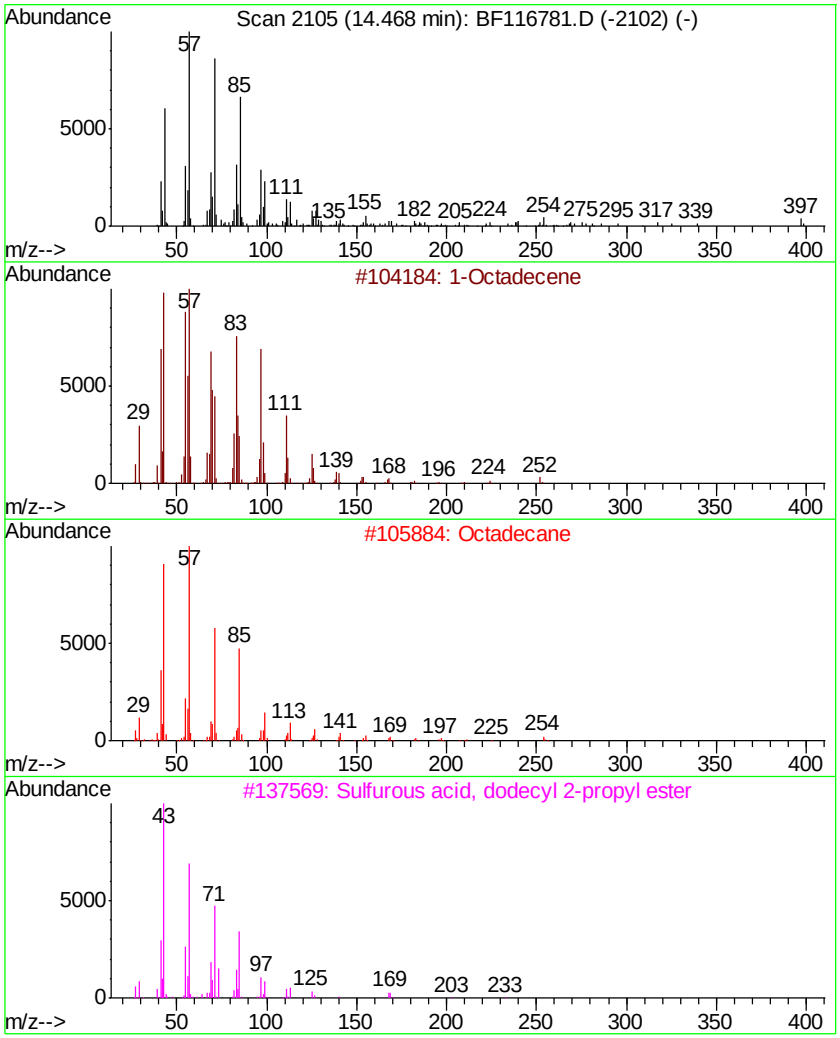
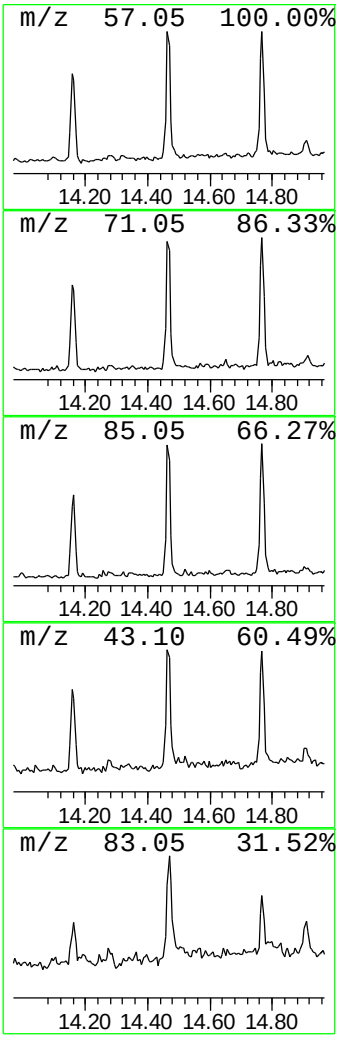
Peak Number 6 1-Octadecene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.47	4.39 ng	212145	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene	252	C18H36	000112-88-9	91
2	Octadecane	254	C18H38	000593-45-3	91
3	Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	91
4	Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	91
5	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	91





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TIC Library : C:\DATABASE\NIST11.L
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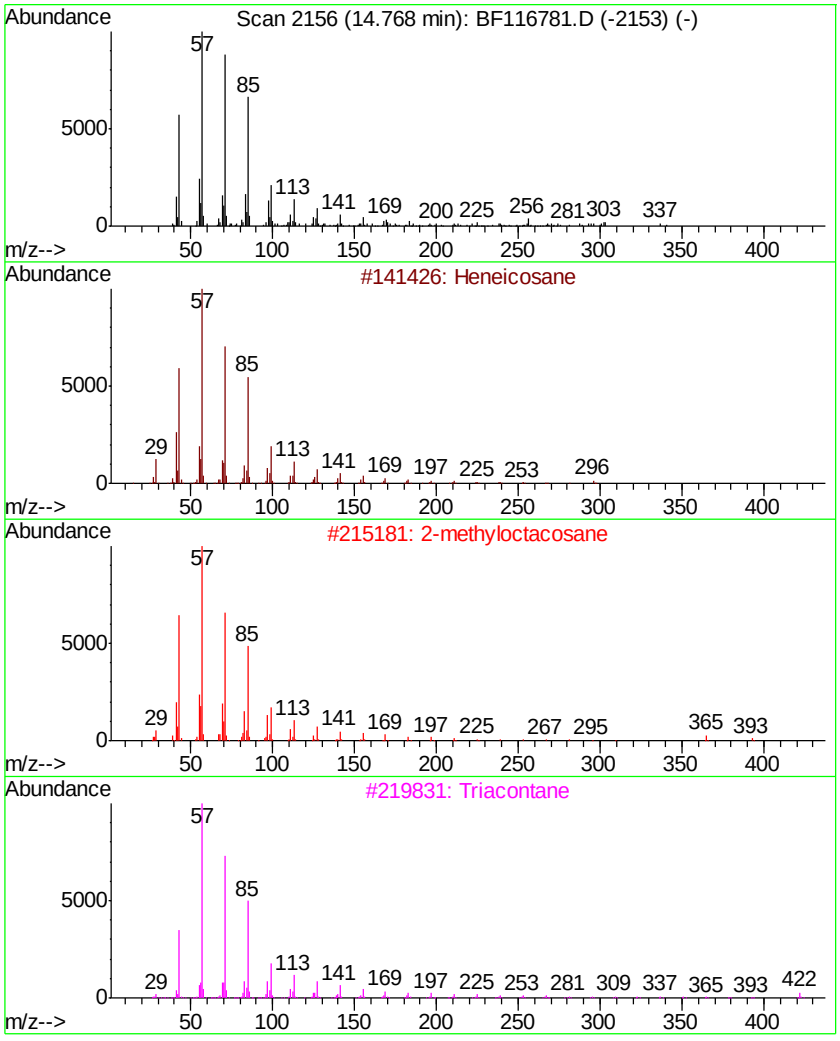
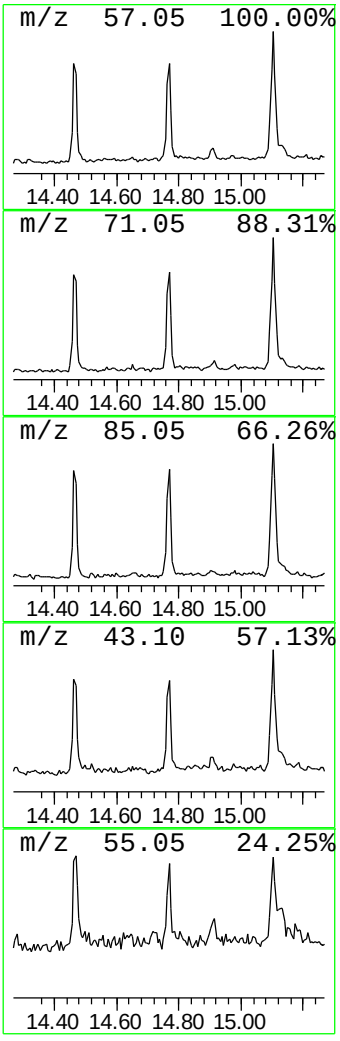
Peak Number 7 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.77	3.94 ng	182286	Perylene-d12	15.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	96
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Triacontane	422	C30H62	000638-68-6	91
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87
5	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	87





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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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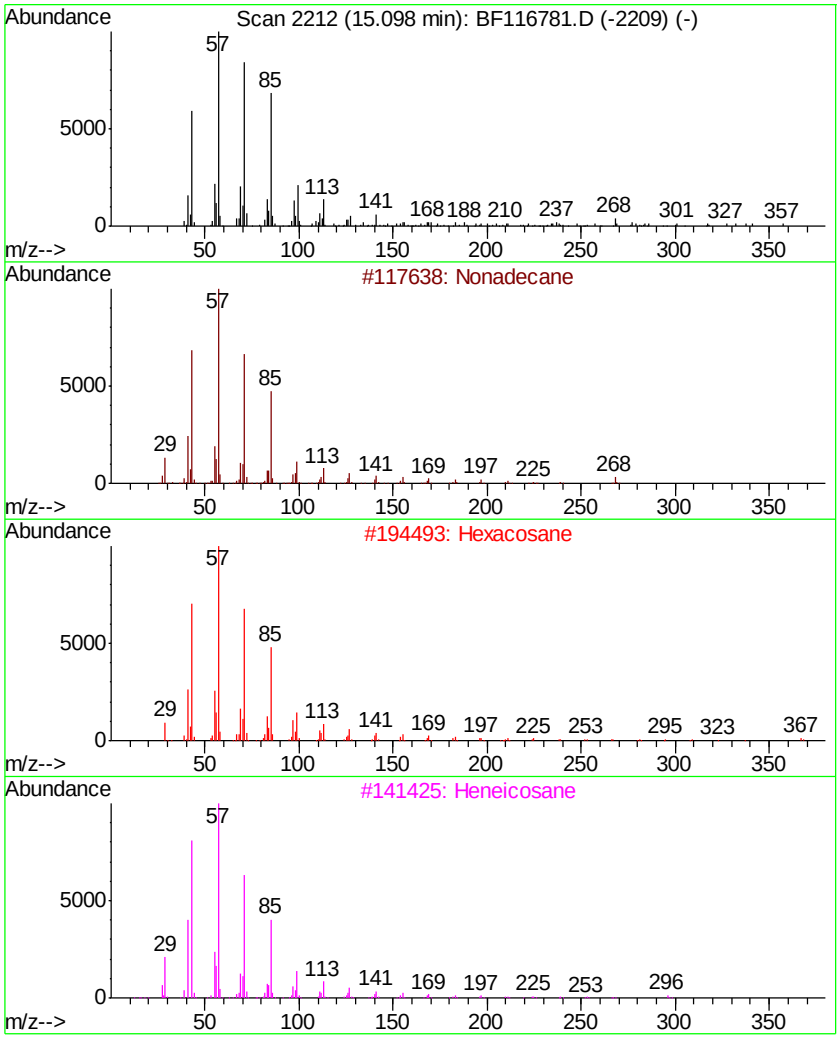
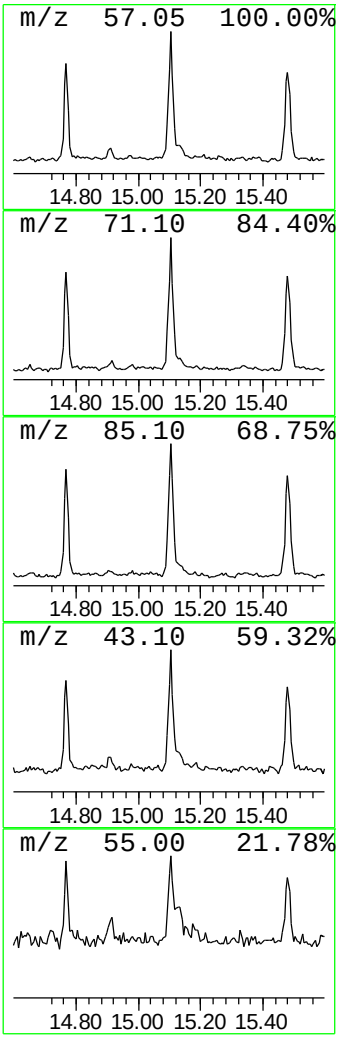
Peak Number 8 Nonadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.10	5.55 ng	256639	Perylene-d12	15.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	91
2	Hexacosane	366	C26H54	000630-01-3	87
3	Heneicosane	296	C21H44	000629-94-7	86
4	Octadecane, 2-methyl-	268	C19H40	001560-88-9	83
5	Decane, 3,6-dimethyl-	170	C12H26	017312-53-7	81





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Data File : BF116781.D
Acq On : 3 Sep 2019 19:12
Operator : HP/JU
Sample : K4554-41
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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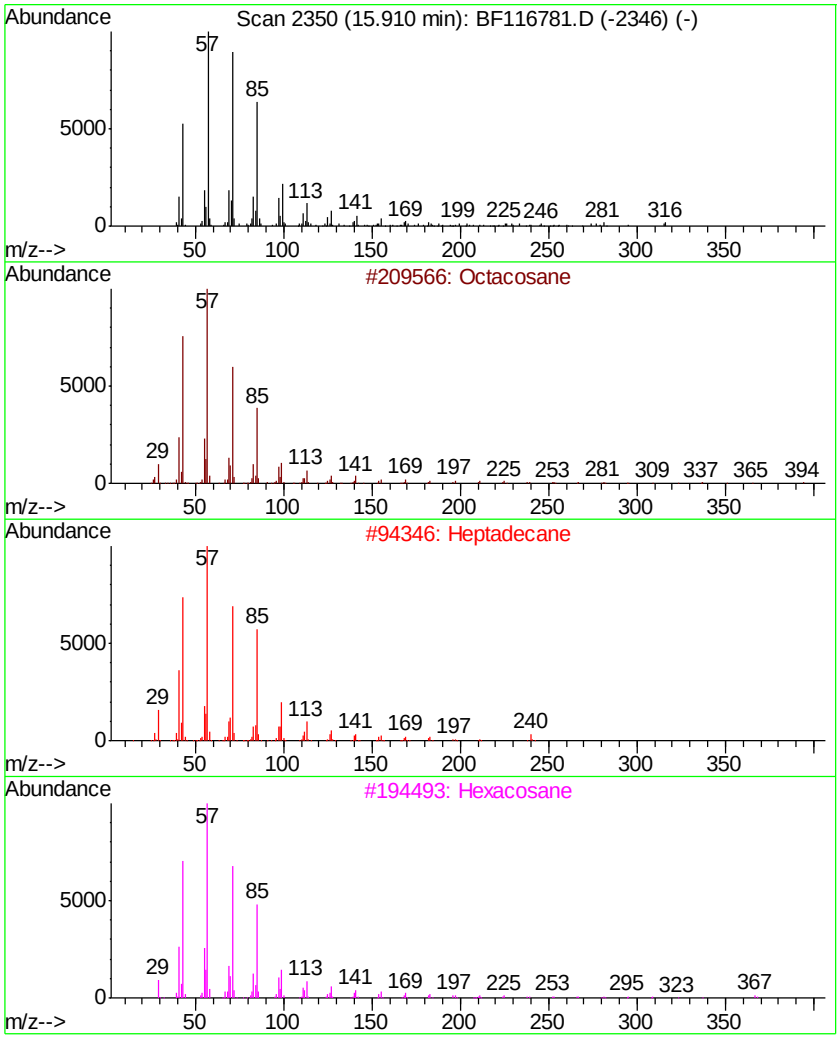
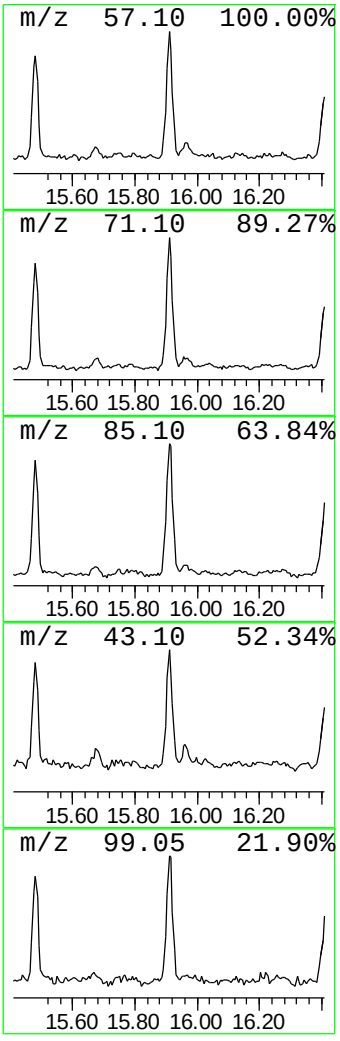
Peak Number 9 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.91	5.73 ng	265005	Perylene-d12	15.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	90
2	Heptadecane	240	C17H36	000629-78-7	90
3	Hexacosane	366	C26H54	000630-01-3	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	6,6-Diethylhoctadecane	310	C22H46	1000360-41-8	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090319\
Data File : BF116781.D
Acq On : 3 Sep 2019 19:12
Operator : HP/JU
Sample : K4554-41
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

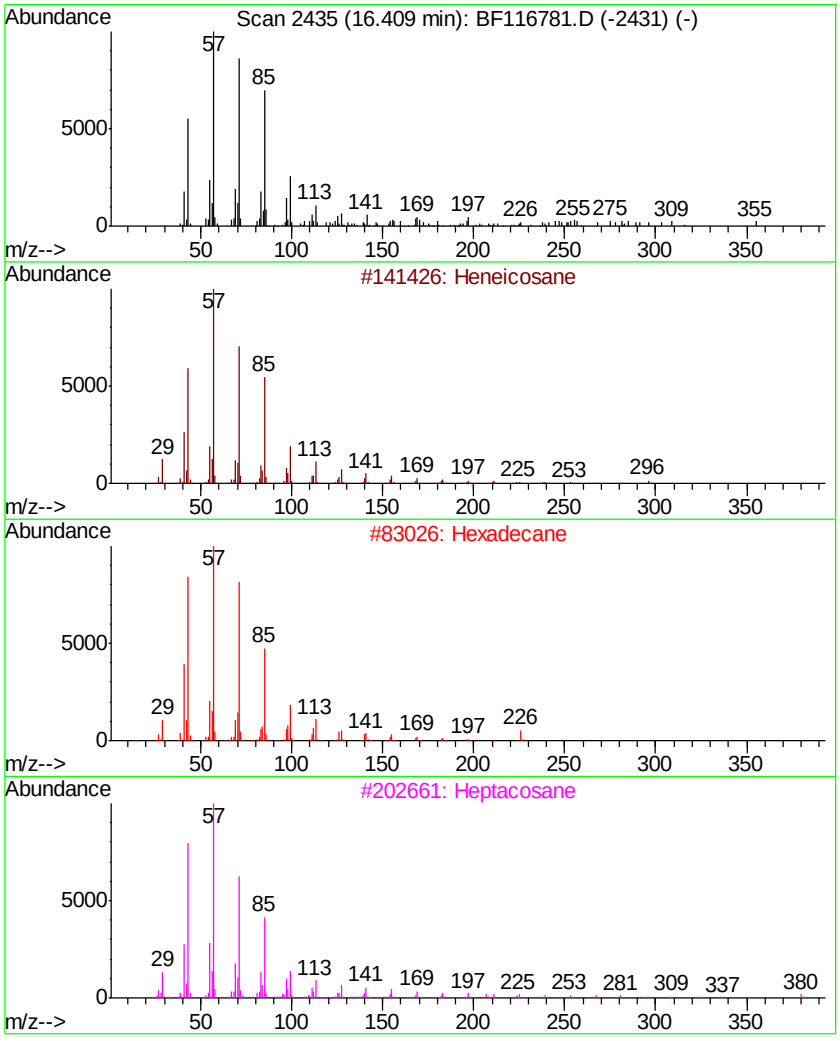
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

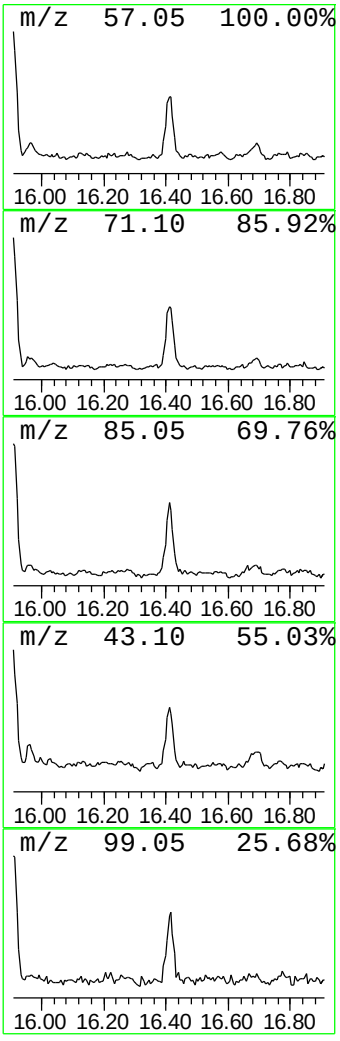
****

Peak Number 10 Heptacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.41	4.12 ng	190832	Perylene-d12	15.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	95
2	Hexadecane	226	C16H34	000544-76-3	90
3	Heptacosane	380	C27H56	000593-49-7	86
4	Pentacosane	352	C25H52	000629-99-2	64
5	Eicosane, 2-methyl-	296	C21H44	001560-84-5	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF090319\
Data File : BF116781.D
Acq On : 3 Sep 2019 19:12
Operator : HP/JU
Sample : K4554-41
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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
unknown6.62	6.62	75.9	ng	2888610	1	6.85	761147	20.0
n-Hexadecanoic acid	11.89	5.5	ng	307255	4	11.36	1110040	20.0
Cetene	13.83	8.9	ng	429995	5	13.99	967580	20.0
Hexadecane	14.16	2.7	ng	132577	5	13.99	967580	20.0
1-Octadecene	14.47	4.4	ng	212145	5	13.99	967580	20.0
Heneicosane	14.77	3.9	ng	182286	6	15.45	925625	20.0
Nonadecane	15.10	5.5	ng	256639	6	15.45	925625	20.0
Octacosane	15.91	5.7	ng	265005	6	15.45	925625	20.0
Heptacosane	16.41	4.1	ng	190832	6	15.45	925625	20.0