LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF052119\
Data File : BF114465.D
Acq On : 21 May 2019 19:23
Operator : JU/SJ
Sample : K2951-15
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-14

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-BF051019.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	5.310	545	548	556	rBV	63424	65193	1.12%	0.137%
2	5.457	570	573	599	rBV	2509662	2688369	46.30%	5.654%
3	6.469	742	745	761	rBV	1663602	1890656	32.56%	3.977%
4	6.604	764	768	775	rBV	4782998	4320790	74.42%	9.088%
5	6.828	803	806	814	rBV	1472341	1218438	20.99%	2.563%
6	6.987	829	833	836	rBV	4493917	4027622	69.37%	8.471%
7	7.392	898	902	905	rBV	3542697	3350352	57.70%	7.047%
8	8.110	1021	1024	1035	rBV	1644247	1580399	27.22%	3.324%
9	9.186	1203	1207	1210	rBV	6242743	5806107	100.00%	12.212%
10	9.580	1271	1274	1279	rVB	101771	91145	1.57%	0.192%
11	9.863	1319	1322	1326	rBV	1688770	1671870	28.80%	3.516%
12	9.898	1326	1328	1334	rVB2	89874	86183	1.48%	0.181%
13	10.075	1354	1358	1362	rBV	261293	246831	4.25%	0.519%
14	10.416	1412	1416	1421	rVB	191819	181155	3.12%	0.381%
15	10.569	1439	1442	1450	rVB	63219	74352	1.28%	0.156%
16	10.657	1453	1457	1472	rVV	3448372	3509251	60.44%	7.381%
17	11.351	1571	1575	1578	rBV	1851925	1737436	29.92%	3.654%
18	11.374	1578	1579	1584	rVV	320802	235387	4.05%	0.495%
19	11.427	1586	1588	1592	rVB	120731	118485	2.04%	0.249%
20	11.586	1611	1615	1620	rBV3	54889	73912	1.27%	0.155%
21	11.857	1657	1661	1662	rBV2	72802	74784	1.29%	0.157%
22	11.874	1662	1664	1672	rVB	565959	579851	9.99%	1.220%
23	11.969	1677	1680	1682	rBV	72471	72825	1.25%	0.153%
24	12.104	1698	1703	1708	rBV4	29537	69656	1.20%	0.147%
25	12.569	1778	1782	1788	rBV	818288	772513	13.31%	1.625%
26	12.657	1791	1797	1805	rBV2	362000	495621	8.54%	1.042%
27	12.798	1815	1821	1827	rVB	557115	590144	10.16%	1.241%
28	12.933	1840	1844	1848	rBV	4682711	4820323	83.02%	10.138%
29	13.827	1993	1996	1998	rBV2	84842	76478	1.32%	0.161%
30	13.851	1998	2000	2007	rVB3	51741	68851	1.19%	0.145%
31	13.992	2019	2024	2027	rBV2	1271547	1466177	25.25%	3.084%
32	14.021	2027	2029	2036	rVB	216304	222472	3.83%	0.468%
33	14.139	2046	2049	2053	rBV	190664	184056	3.17%	0.387%
34	14.445	2098	2101	2106	rBV	398013	348666	6.01%	0.733%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF052119\
Data File : BF114465.D
Acq On : 21 May 2019 19:23
Operator : JU/SJ
Sample : K2951-15
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-14

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-BF051019.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.751	2149	2153	2158	rVB	538876	518938	8.94%	1.091%
36	15.039	2198	2202	2205	rBV	172663	267591	4.61%	0.563%
37	15.080	2205	2209	2214	rVB2	595346	694466	11.96%	1.461%
38	15.339	2250	2253	2260	rVB	100869	124441	2.14%	0.262%
39	15.404	2261	2264	2268	rBV	86218	97813	1.68%	0.206%
40	15.462	2268	2274	2284	rVV2	1220106	1876945	32.33%	3.948%
41	15.880	2340	2345	2352	rVB	390472	569059	9.80%	1.197%
42	16.374	2424	2429	2440	rVB2	195781	346587	5.97%	0.729%
43	16.951	2522	2527	2534	rVB4	105271	233067	4.01%	0.490%

Sum of corrected areas: 47545257

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF052119\
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Acq On : 21 May 2019 19:23
Operator : JU/SJ
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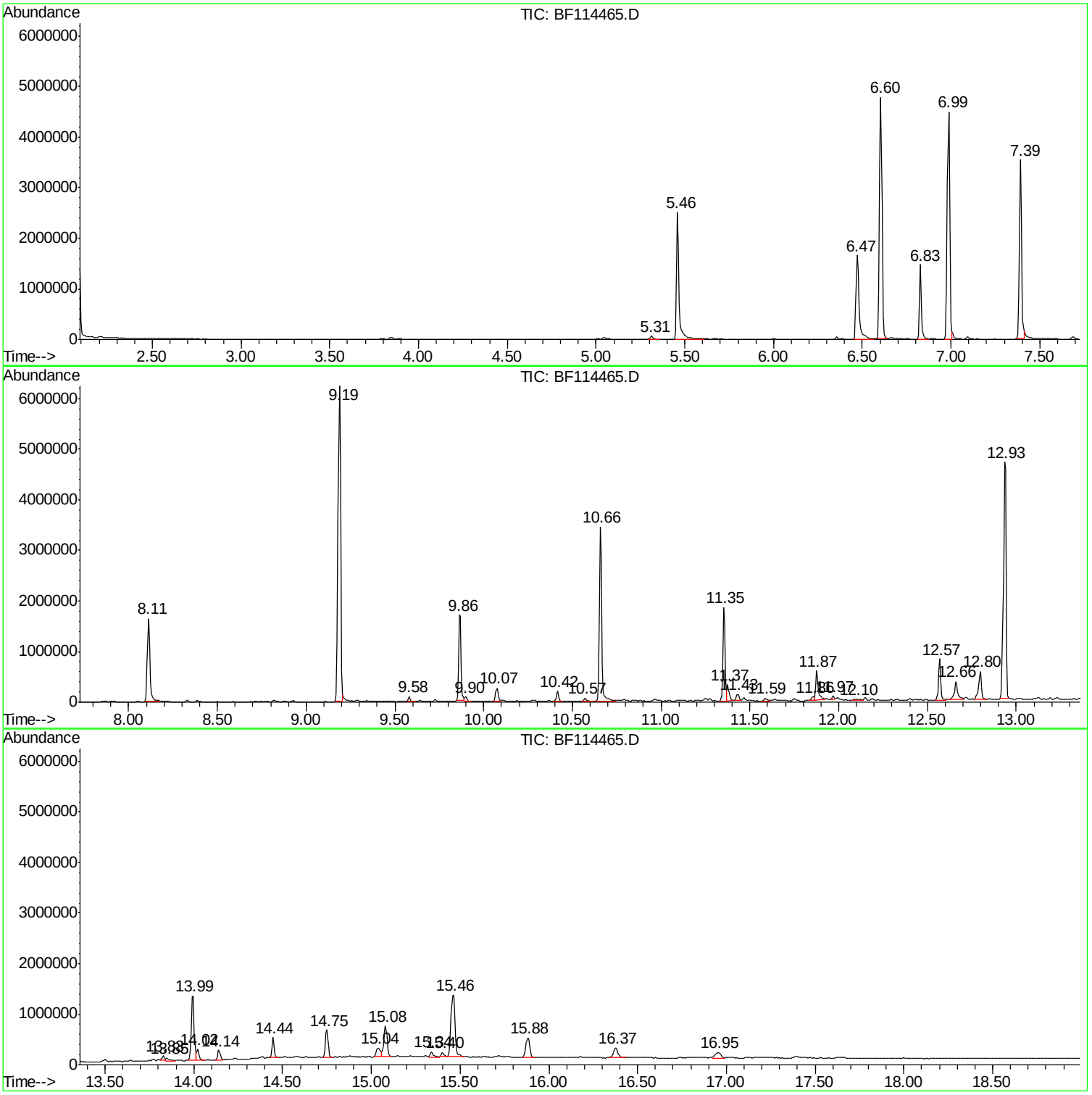
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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\BF052119\
Data File : BF114465.D
Acq On : 21 May 2019 19:23
Operator : JU/SJ
Sample : K2951-15
Misc :
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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

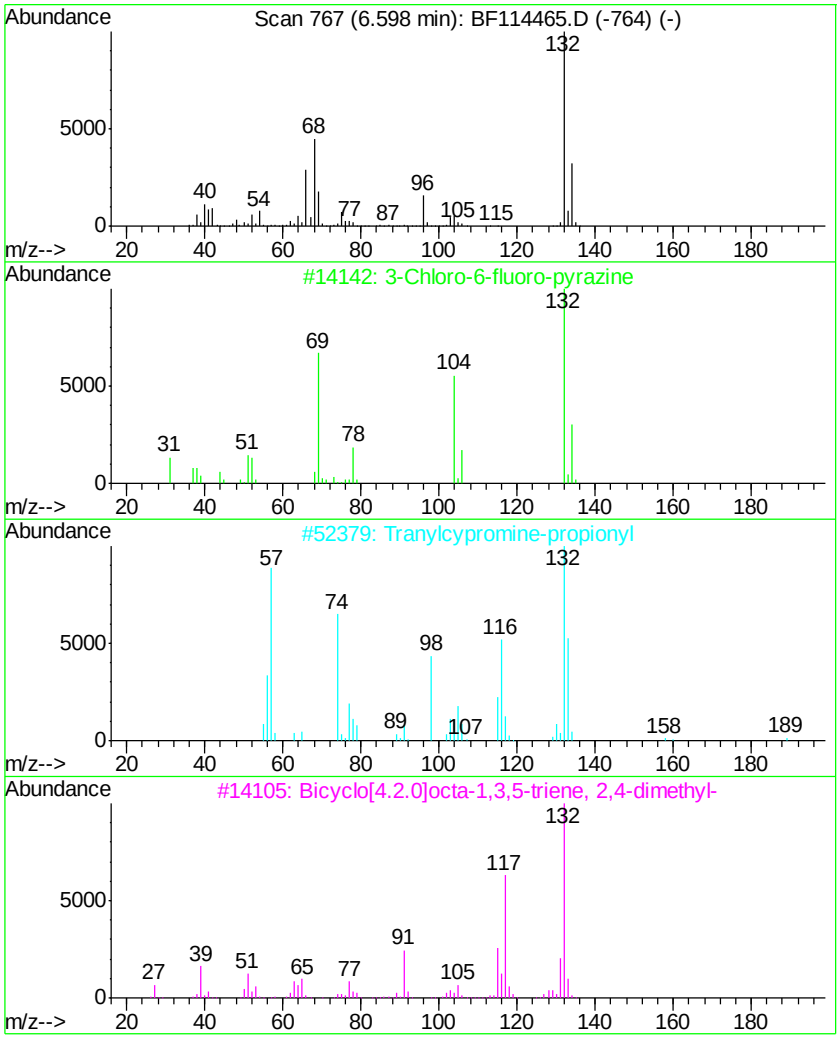
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

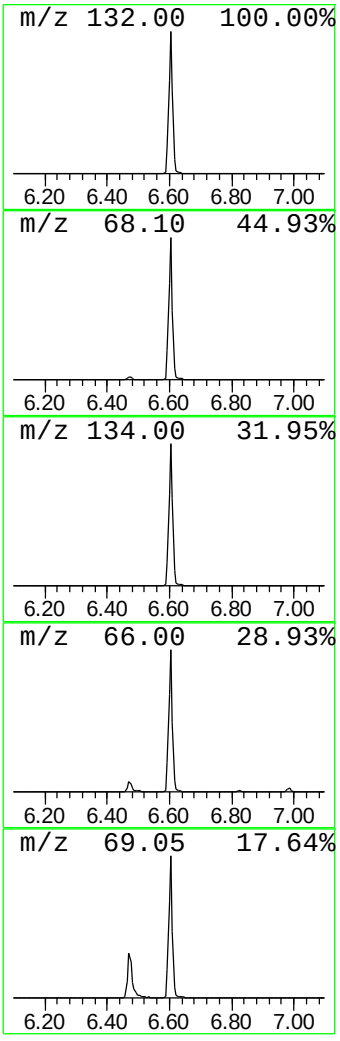
****

Peak Number 1 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	70.92 ng	4320790	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
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	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Library Search Compound Report

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Operator : JU/SJ
Sample : K2951-15
Misc :
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Instrument : BNA_F
ClientSampleId : TP-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

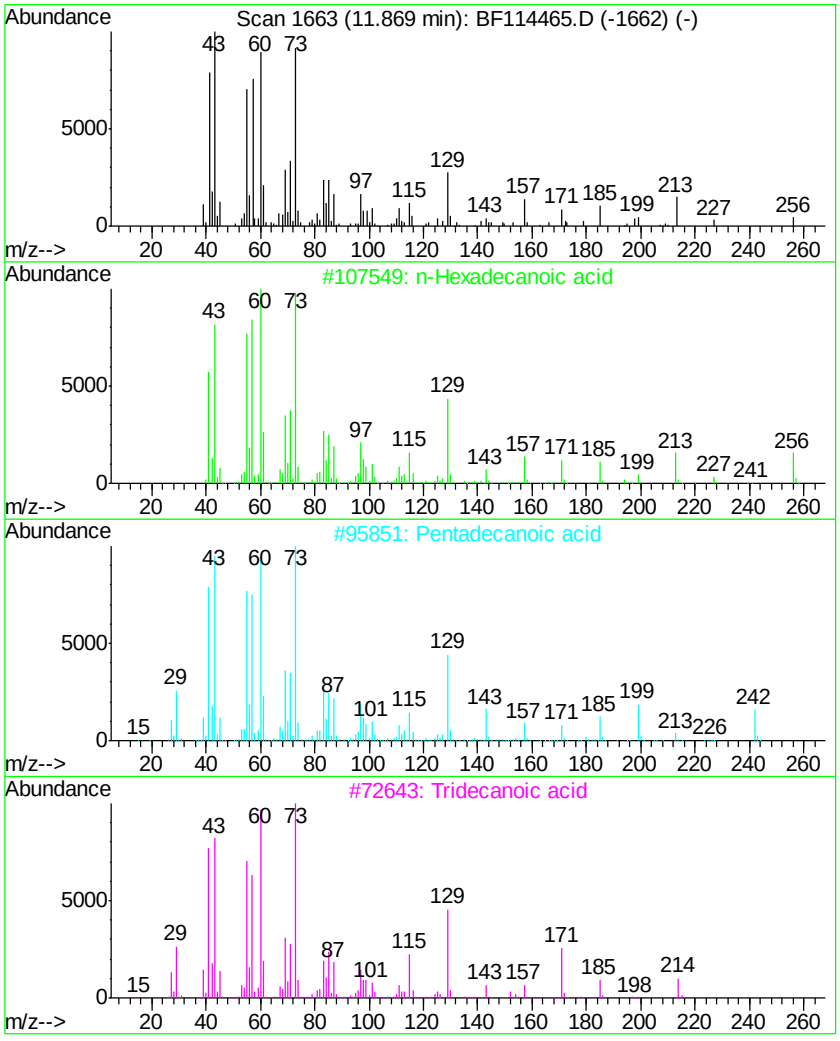
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

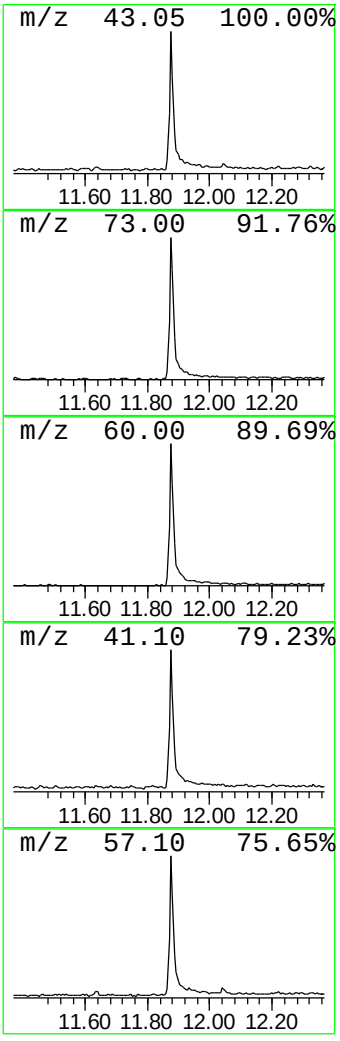
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	6.67 ng	579851	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	78





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF052119\
Data File : BF114465.D
Acq On : 21 May 2019 19:23
Operator : JU/SJ
Sample : K2951-15
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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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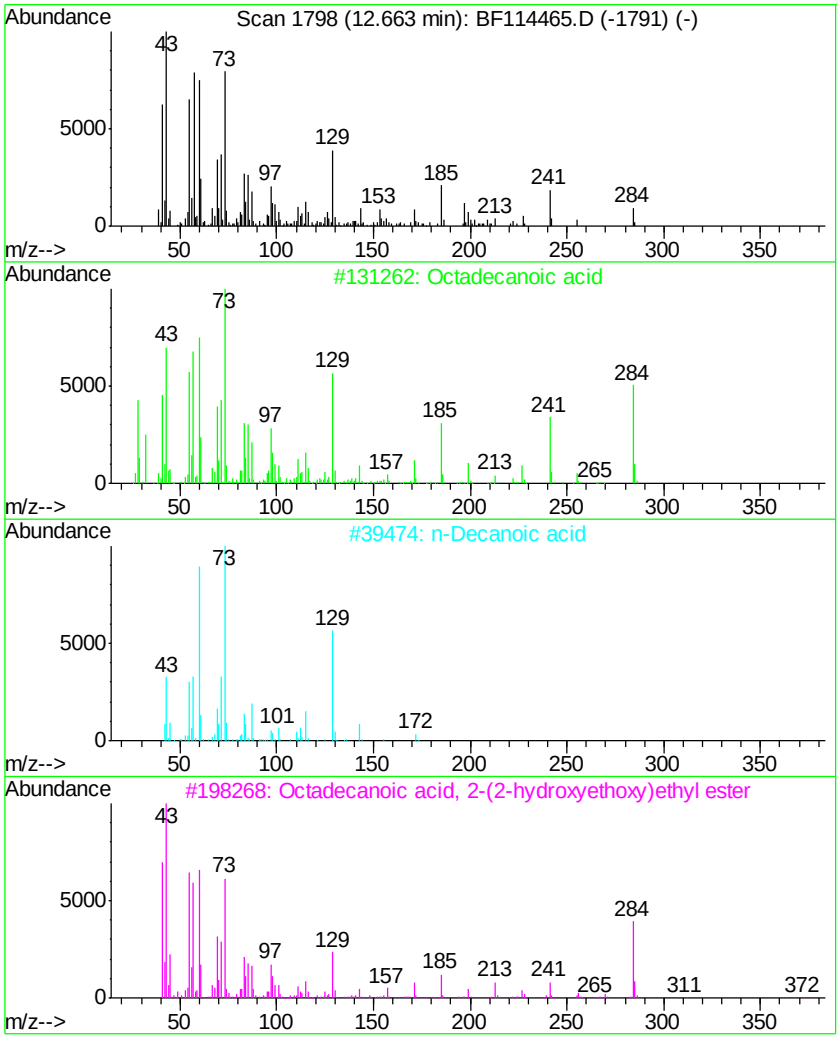
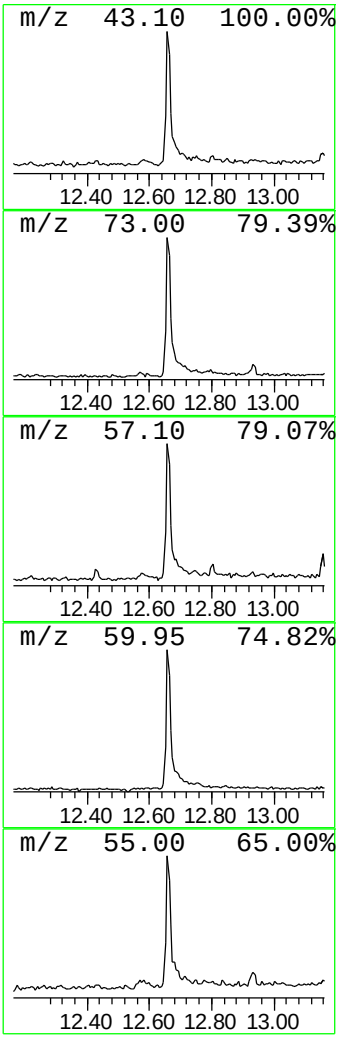
Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.66	5.71 ng	495621	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Decanoic acid	172	C10H20O2	000334-48-5	91
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	74





Library Search Compound Report

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Data File : BF114465.D
Acq On : 21 May 2019 19:23
Operator : JU/SJ
Sample : K2951-15
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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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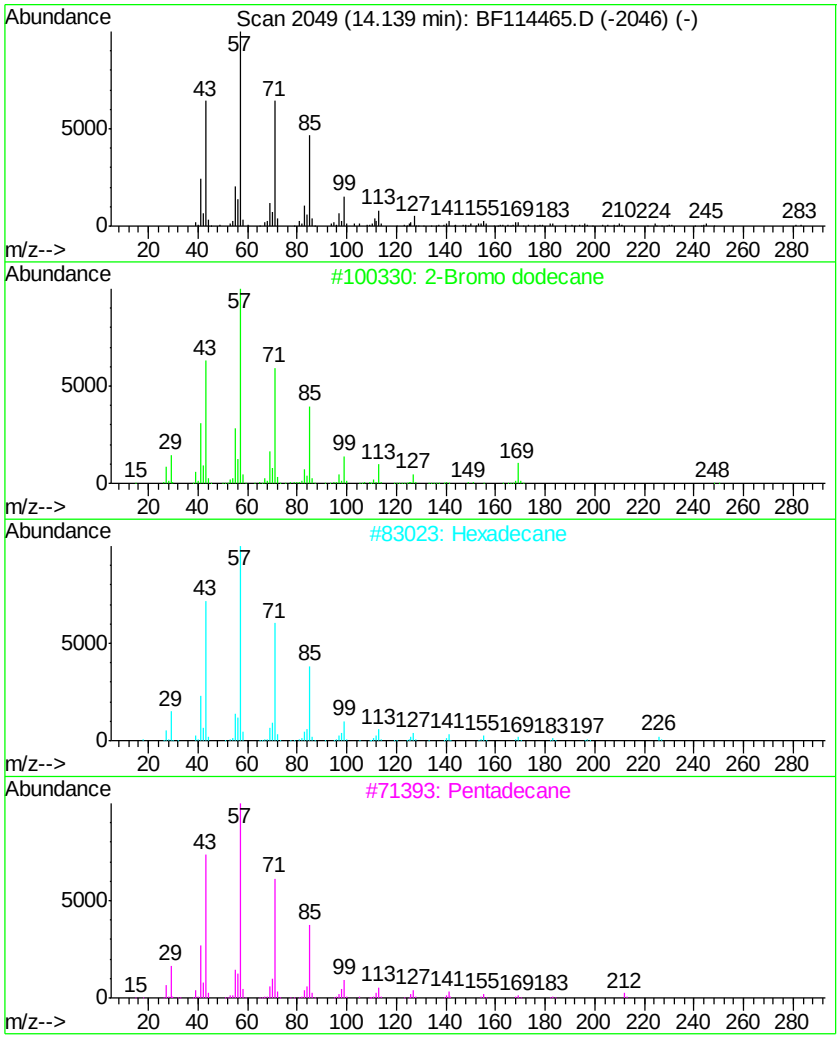
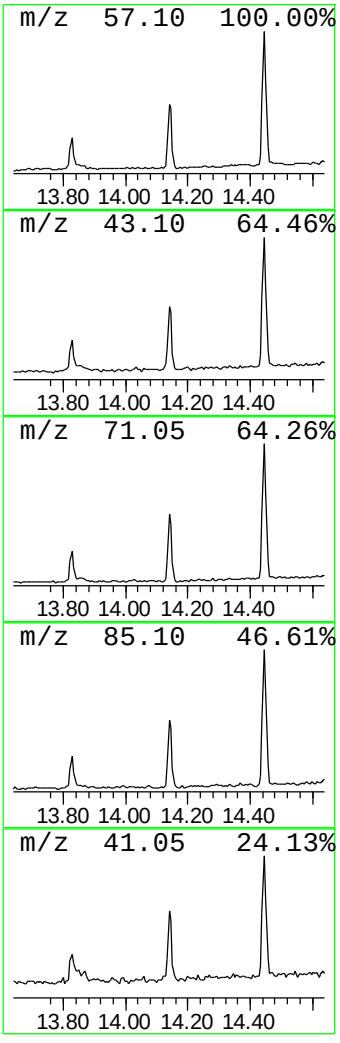
Peak Number 5 2-Bromo dodecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.14	2.51 ng	184056	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromo dodecane	248	C12H25Br	013187-99-0	89
2	Hexadecane	226	C16H34	000544-76-3	86
3	Pentadecane	212	C15H32	000629-62-9	86
4	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86
5	Heptacosane	380	C27H56	000593-49-7	76





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF052119\
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Operator : JU/SJ
Sample : K2951-15
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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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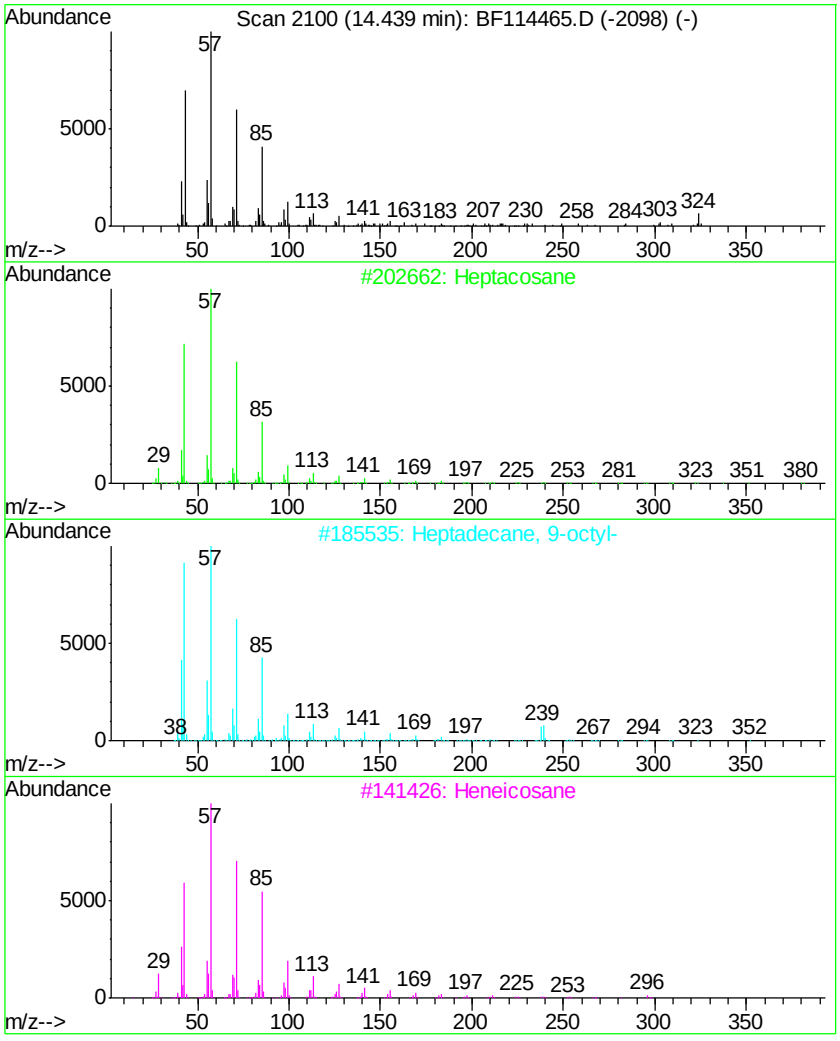
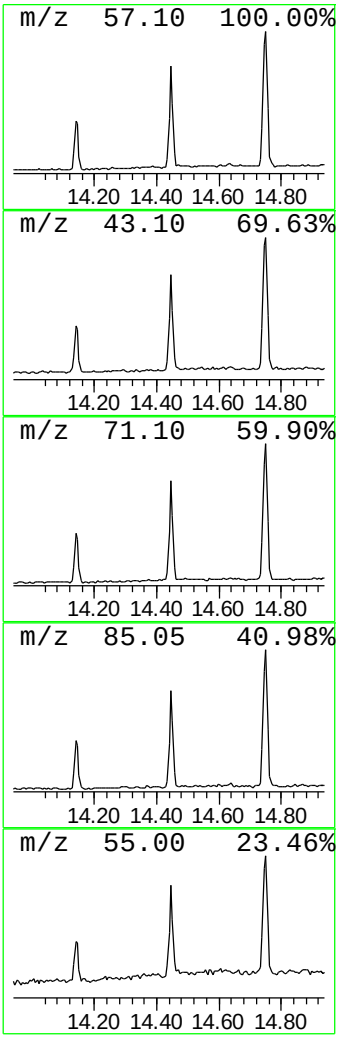
Peak Number 6 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.44	4.76 ng	348666	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Docosane, 11-butyl-	366	C26H54	013475-76-8	91
5	Hexacosane	366	C26H54	000630-01-3	91





Library Search Compound Report

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Operator : JU/SJ
Sample : K2951-15
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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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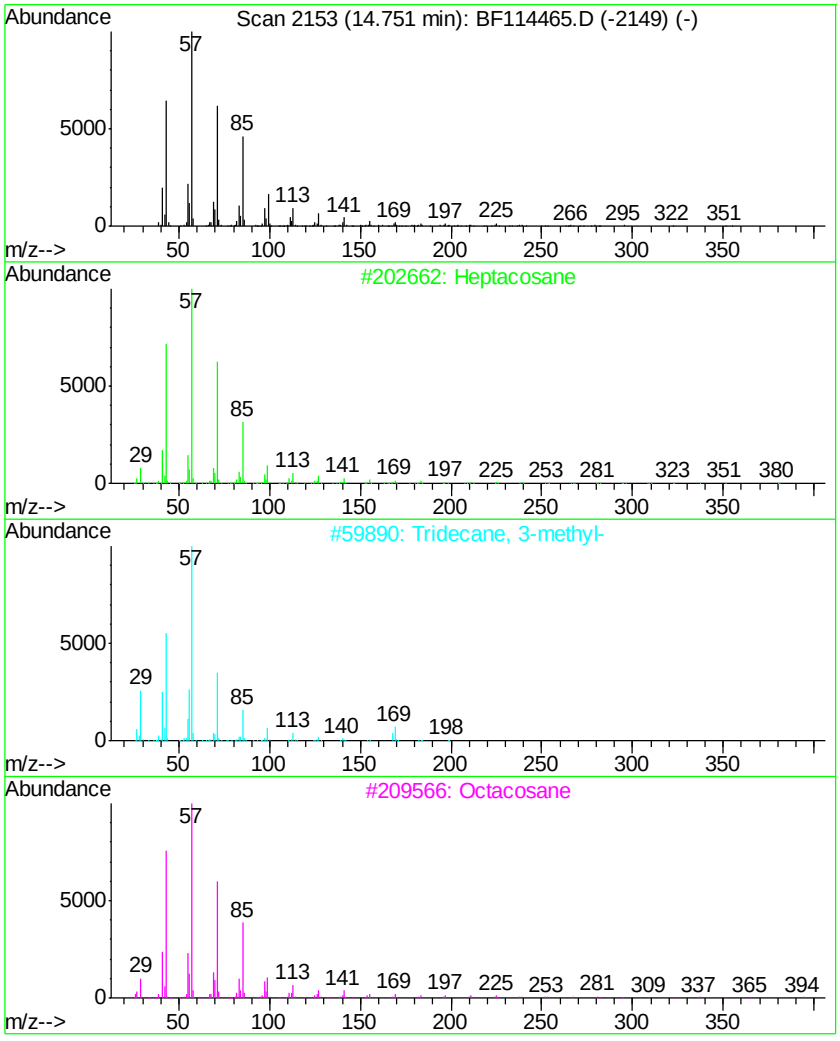
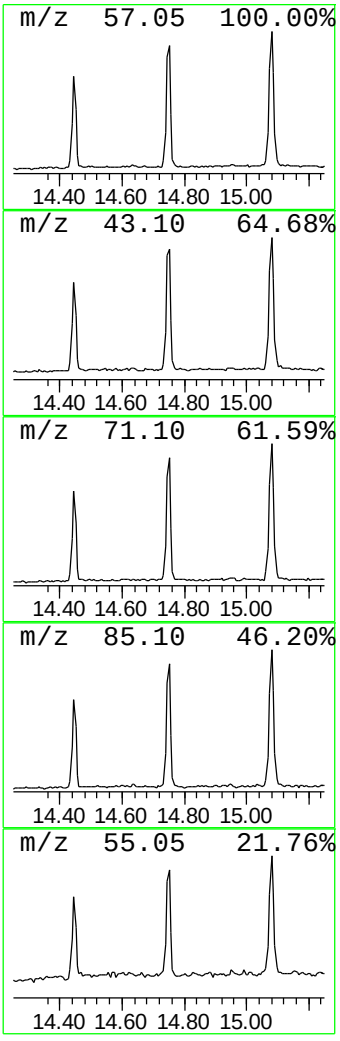
Peak Number 7 Tridecane, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.75	5.53 ng	518938	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Tridecane, 3-methyl-	198	C14H30	006418-41-3	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Hexacosane	366	C26H54	000630-01-3	91





Library Search Compound Report

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Sample : K2951-15
Misc :
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Instrument : BNA_F
ClientSampleId : TP-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

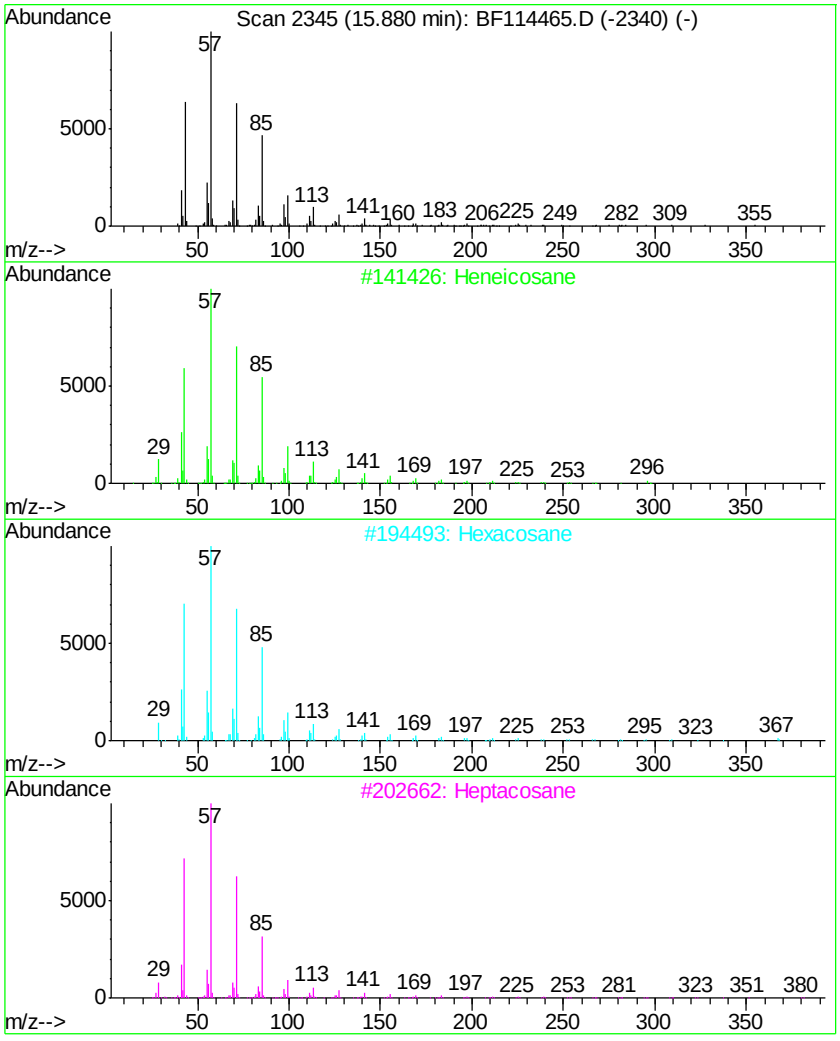
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

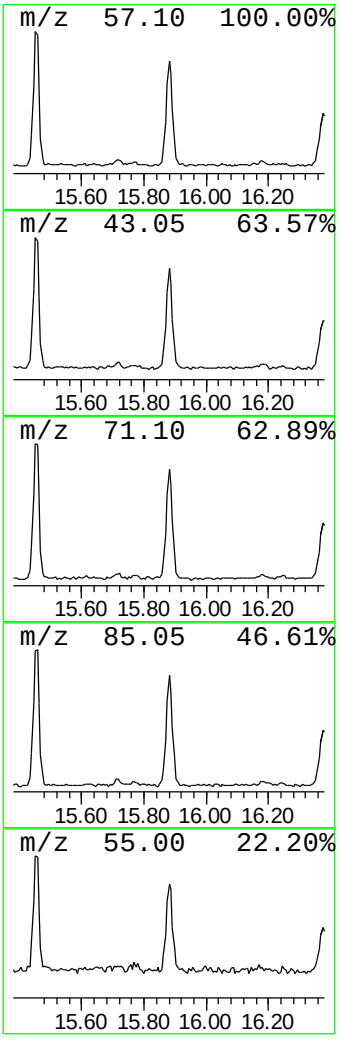
****

Peak Number 8 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.88	6.06 ng	569059	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Octadecane, 2-methyl-	268	C19H40	001560-88-9	90





Library Search Compound Report

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Operator : JU/SJ
Sample : K2951-15
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

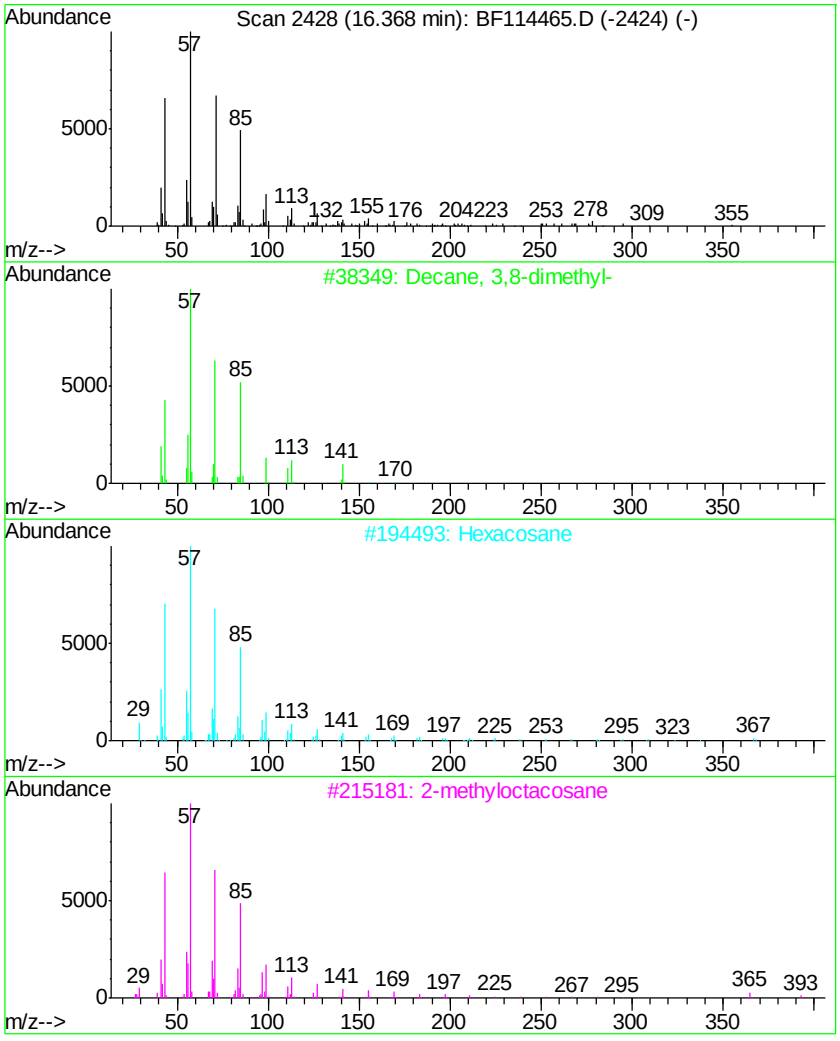
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

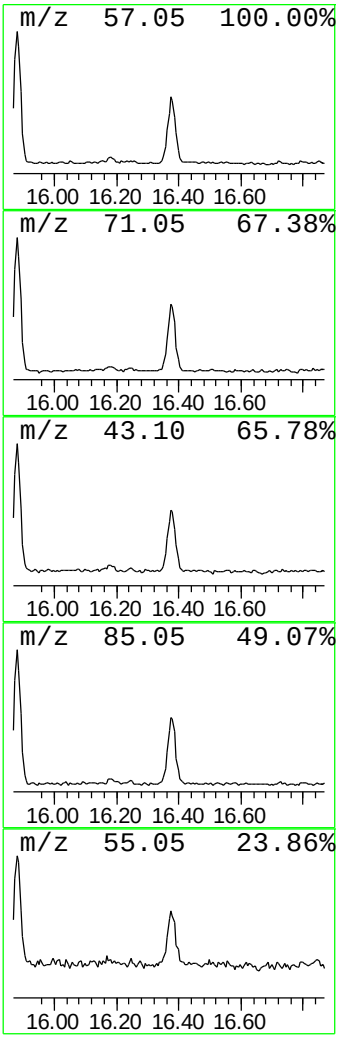
****

Peak Number 9 Decane, 3,8-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.37	3.69 ng	346587	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	87
2	Hexacosane	366	C26H54	000630-01-3	87
3	2-methyloctacosane	408	C29H60	1000376-72-8	87
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5	Heptacosane	380	C27H56	000593-49-7	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF052119\
Data File : BF114465.D
Acq On : 21 May 2019 19:23
Operator : JU/SJ
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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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
unknown6.60	6.60	70.9	ng	4320790	1	6.83	1218440	20.0
n-Hexadecanoic acid	11.87	6.7	ng	579851	4	11.35	1737440	20.0
Octadecanoic acid	12.66	5.7	ng	495621	4	11.35	1737440	20.0
2-Bromo dodecane	14.14	2.5	ng	184056	5	14.00	1466180	20.0
Heptacosane	14.44	4.8	ng	348666	5	14.00	1466180	20.0
Tridecane, 3-methyl-	14.75	5.5	ng	518938	6	15.46	1876950	20.0
Heneicosane	15.88	6.1	ng	569059	6	15.46	1876950	20.0
Decane, 3,8-dimet...	16.37	3.7	ng	346587	6	15.46	1876950	20.0