LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021419\
Data File : BF112572.D
Acq On : 14 Feb 2019 17:14
Operator : JU/SJ
Sample : K1458-11 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-7

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-BF012519.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	5.040	498	502	511	rBV	29392	43136	4.20%	0.350%
2	5.463	571	574	595	rBV	651994	803753	78.22%	6.519%
3	6.481	743	747	765	rBV	658766	930256	90.53%	7.545%
4	6.604	765	768	776	rVV	1001402	935779	91.07%	7.590%
5	6.828	803	806	814	rBV	653187	581818	56.62%	4.719%
6	6.987	829	833	844	rBV	797707	714286	69.52%	5.793%
7	7.098	848	852	855	rBV5	13355	15940	1.55%	0.129%
8	7.222	867	873	876	rBV3	10294	15003	1.46%	0.122%
9	7.392	899	902	911	rBV	519261	536628	52.23%	4.352%
10	7.745	960	962	966	rVB2	15689	16231	1.58%	0.132%
11	8.110	1021	1024	1031	rBV	701805	705705	68.68%	5.724%
12	8.163	1031	1033	1036	rVB	24357	26686	2.60%	0.216%
13	8.398	1065	1073	1079	rBV6	14700	31643	3.08%	0.257%
14	8.528	1092	1095	1097	rBV	26691	21954	2.14%	0.178%
15	8.651	1112	1116	1118	rBV3	9584	11346	1.10%	0.092%
16	8.792	1137	1140	1145	rVB4	8357	11318	1.10%	0.092%
17	8.992	1170	1174	1176	rBV4	8462	12250	1.19%	0.099%
18	9.104	1190	1193	1195	rBV2	10324	10619	1.03%	0.086%
19	9.128	1195	1197	1203	rVB3	27373	22128	2.15%	0.179%
20	9.186	1203	1207	1217	rBV	1077890	1027527	100.00%	8.334%
21	9.263	1217	1220	1224	rVV5	18081	21862	2.13%	0.177%
22	9.457	1251	1253	1258	rBV6	8092	10643	1.04%	0.086%
23	9.581	1269	1274	1280	rBV	106968	117395	11.43%	0.952%
24	9.728	1297	1299	1302	rBV3	11538	11136	1.08%	0.090%
25	9.775	1304	1307	1309	rVV2	17916	13721	1.34%	0.111%
26	9.869	1319	1323	1338	rVB	925083	842978	82.04%	6.837%
27	10.292	1392	1395	1397	rVB2	11486	12433	1.21%	0.101%
28	10.510	1429	1432	1437	rVB3	10015	11408	1.11%	0.093%
29	10.663	1455	1458	1467	rBV	599237	587488	57.17%	4.765%
30	10.775	1472	1477	1480	rVB2	15988	19559	1.90%	0.159%
31	11.239	1553	1556	1562	rBV5	12841	13448	1.31%	0.109%
32	11.357	1572	1576	1586	rBV	842541	810608	78.89%	6.574%
33	11.833	1653	1657	1659	rBV5	10993	11221	1.09%	0.091%
34	11.874	1659	1664	1674	rBV3	95017	133331	12.98%	1.081%

LSC Area Percent Report

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Sample : K1458-11 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-7

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-BF012519.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.163	1710	1713	1716	rVB5	16587	13538	1.32%	0.110%
36	12.533	1774	1776	1781	rVB6	13430	11897	1.16%	0.096%
37	12.604	1781	1788	1794	rBV8	30968	80598	7.84%	0.654%
38	12.663	1795	1798	1806	rBV6	38554	71629	6.97%	0.581%
39	12.727	1806	1809	1811	rBV2	49312	49342	4.80%	0.400%
40	12.804	1820	1822	1829	rVB5	25142	41582	4.05%	0.337%
41	12.863	1829	1832	1834	rBV4	19831	24635	2.40%	0.200%
42	12.939	1841	1845	1848	rBV	1014036	910056	88.57%	7.381%
43	13.827	1994	1996	2000	rBV3	89739	118095	11.49%	0.958%
44	14.004	2023	2026	2031	rBV	690139	712033	69.30%	5.775%
45	14.145	2048	2050	2053	rBV	61357	51254	4.99%	0.416%
46	14.451	2099	2102	2105	rBV	111058	102680	9.99%	0.833%
47	14.751	2151	2153	2156	rVB	157418	141034	13.73%	1.144%
48	15.086	2207	2210	2219	rVB	200465	249223	24.25%	2.021%
49	15.462	2271	2274	2275	rBV	148810	155537	15.14%	1.261%
50	15.486	2275	2278	2284	rVB	398740	505387	49.18%	4.099%

Sum of corrected areas: 12329757

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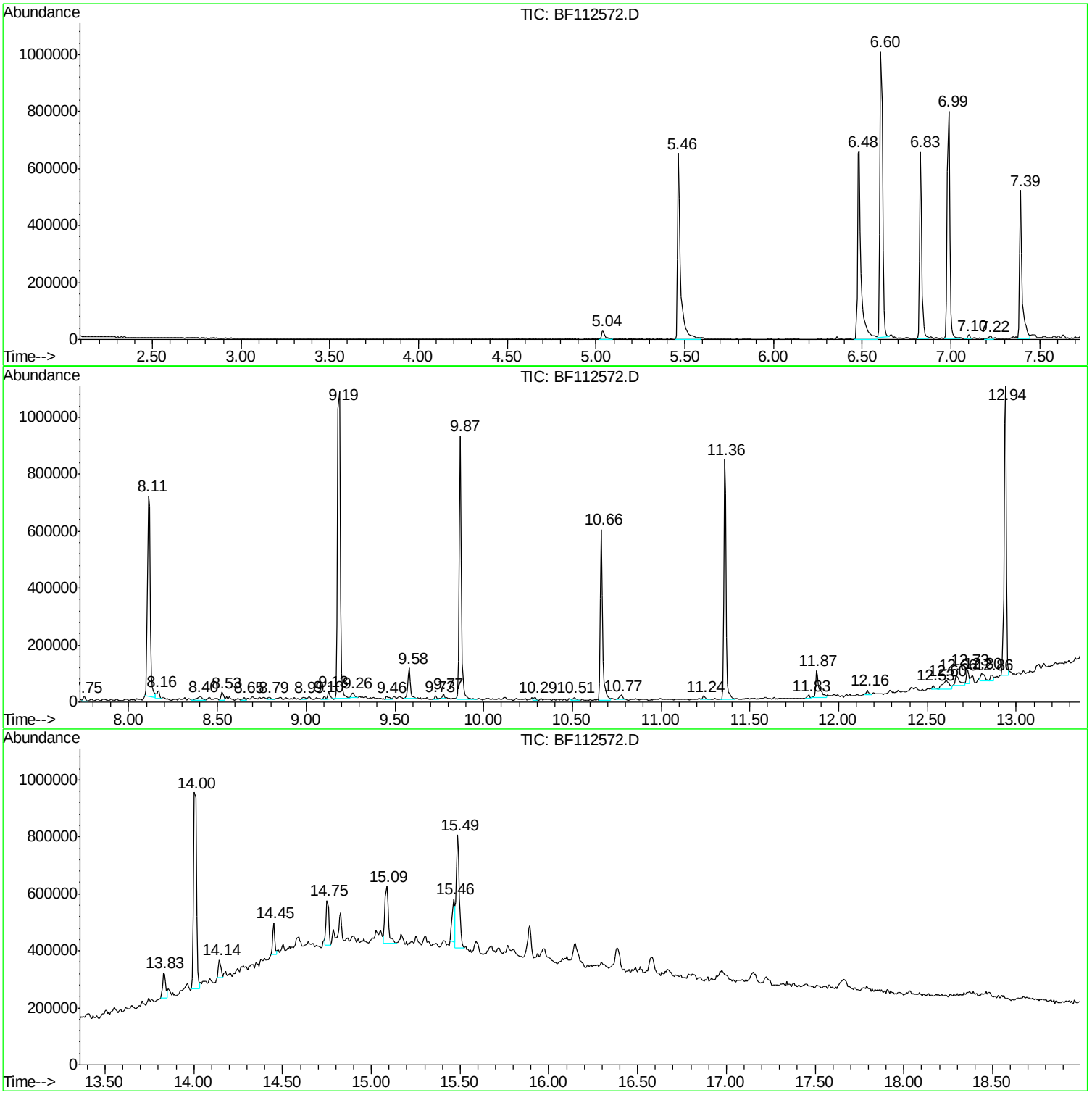
Instrument :
BNA_F
ClientSampleId :
SB-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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 : BF112572.D
Acq On : 14 Feb 2019 17:14
Operator : JU/SJ
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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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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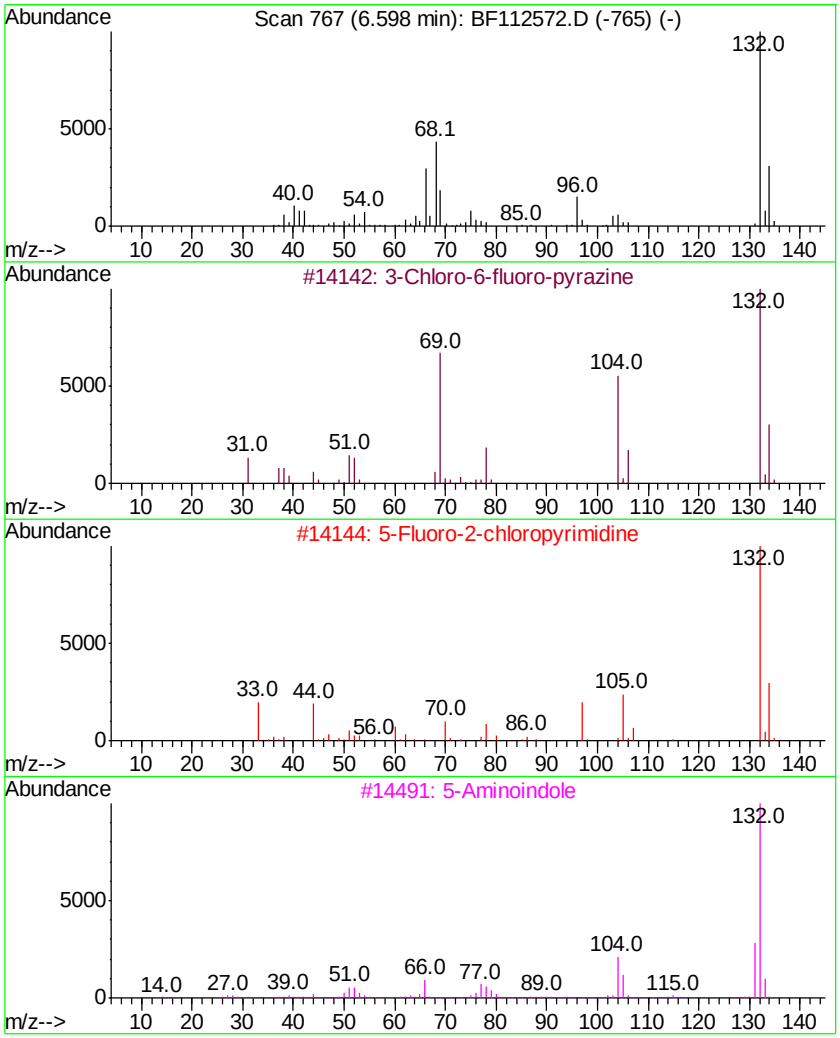
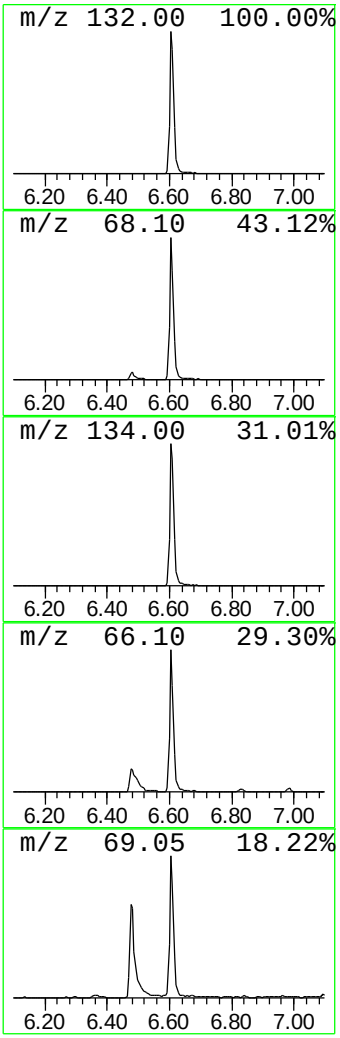
Peak Number 1 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	32.17 ng	935779	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	35
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Misc :
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Instrument : BNA_F
ClientSampleId : SB-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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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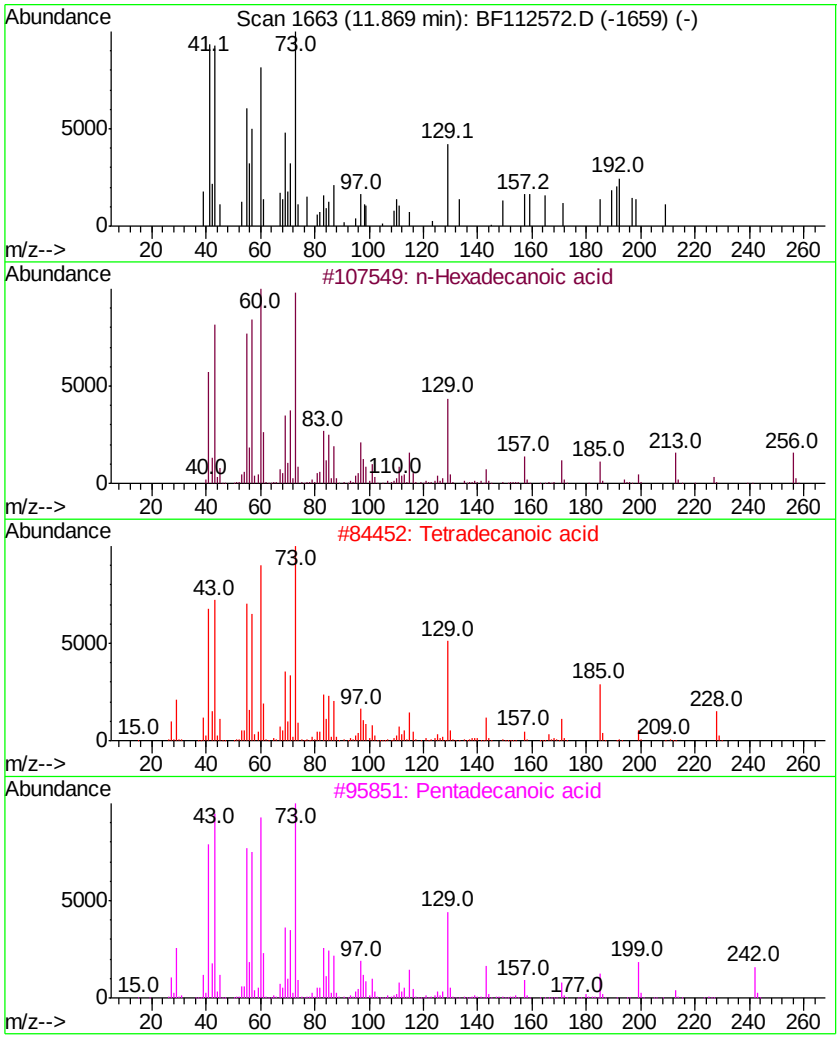
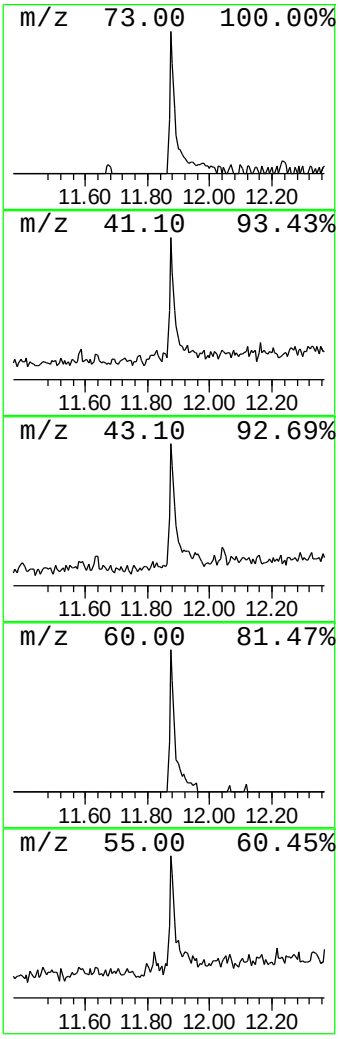
Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	3.29 ng	133331	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Dodecanoic acid	200	C12H24O2	000143-07-7	64
5	.alpha.-d-Riboside, 1-O-dodecyl-	318	C17H34O5	1000154-76-8	47





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : SB-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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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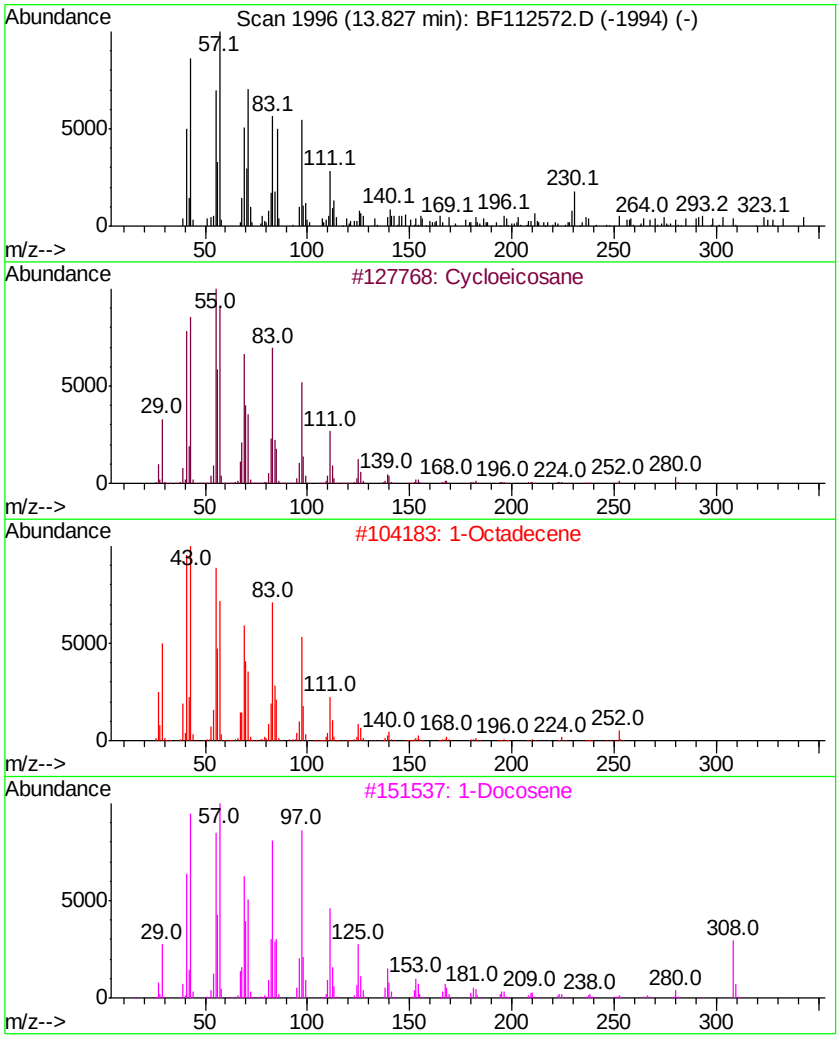
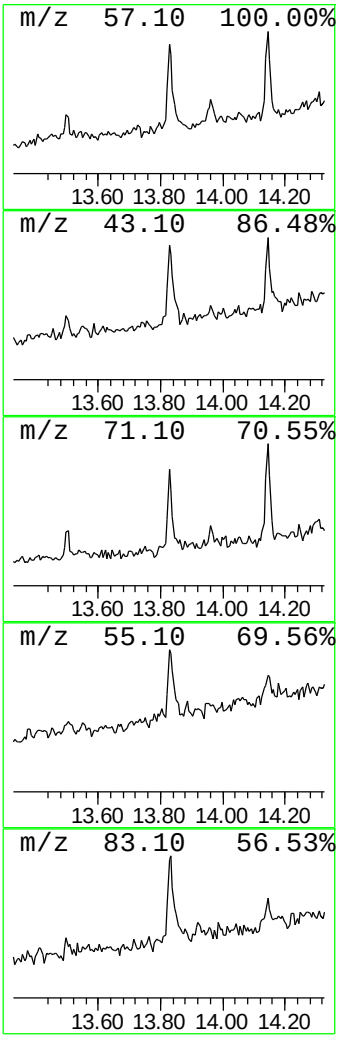
Peak Number 4 Cycloeicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	3.32 ng	118095	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloeicosane	280	C20H40	000296-56-0	95
2	1-Octadecene	252	C18H36	000112-88-9	89
3	1-Docosene	308	C22H44	001599-67-3	87
4	Cyclotetradecane	196	C14H28	000295-17-0	86
5	Oxalic acid, octadecyl propyl ester	384	C23H44O4	1000309-27-0	83





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Sample : K1458-11 2X
Misc :
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Instrument : BNA_F
ClientSampleId : SB-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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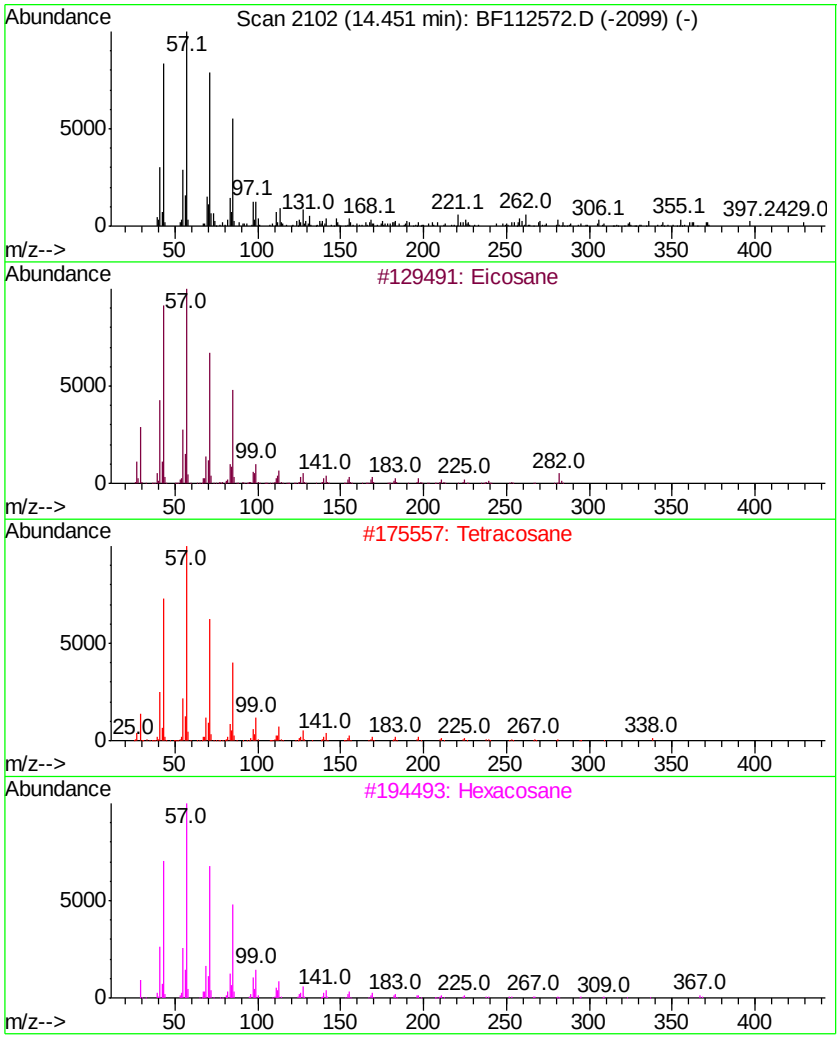
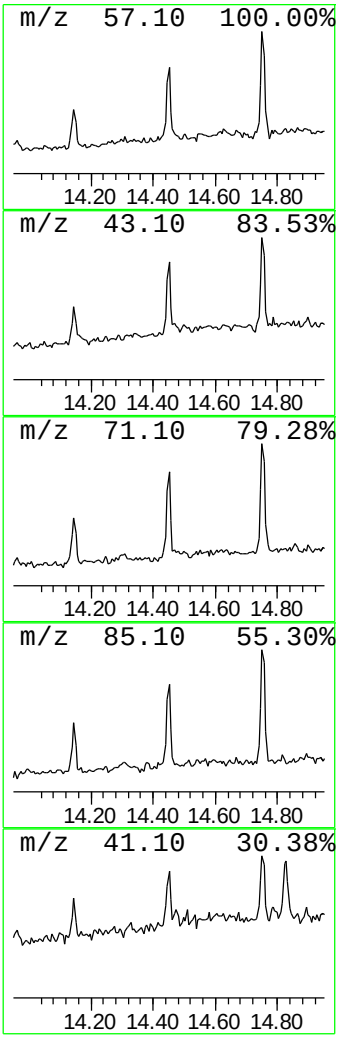
Peak Number 5 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	2.88 ng	102680	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Tetracosane	338	C24H50	000646-31-1	87
3	Hexacosane	366	C26H54	000630-01-3	87
4	Tridecane, 3-ethyl-	212	C15H32	013286-73-2	87
5	Docosane, 11-decyl-	451	C32H66	055401-55-3	87





Library Search Compound Report

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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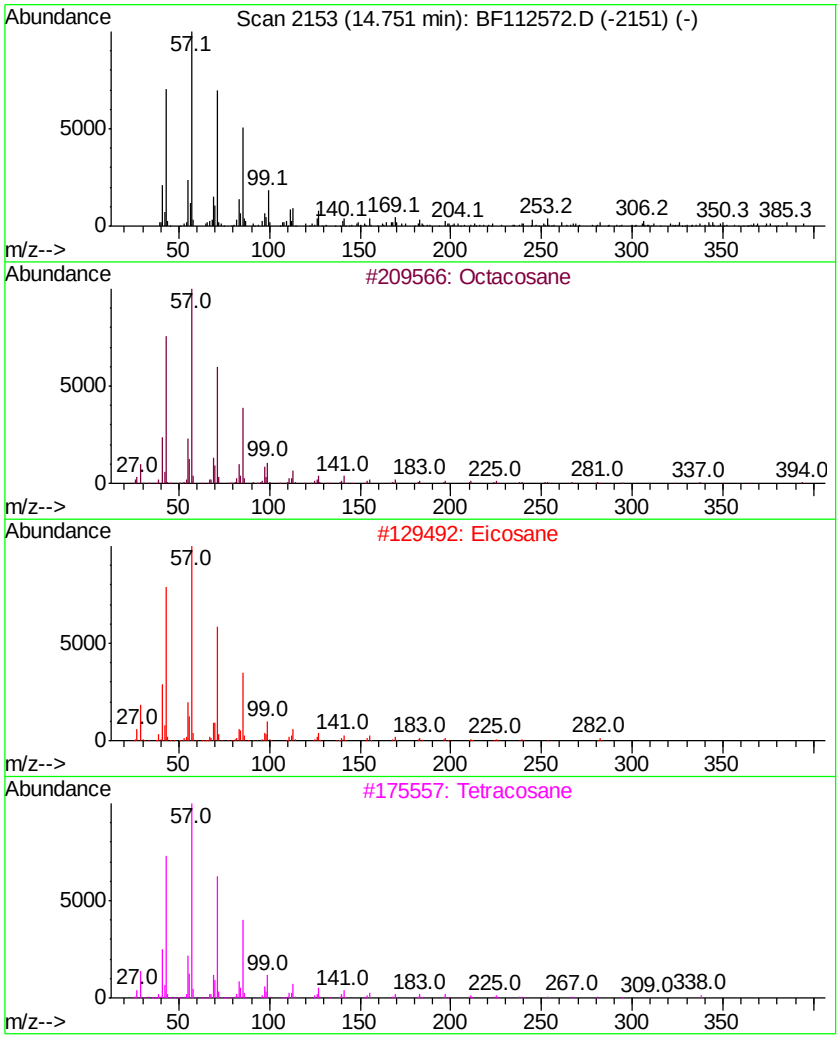
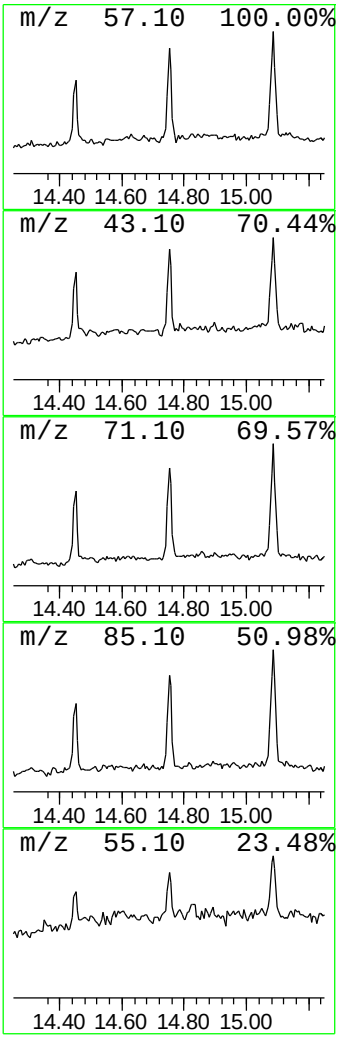
Peak Number 6 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.75	5.58 ng	141034	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	93
2	Eicosane	282	C20H42	000112-95-8	89
3	Tetracosane	338	C24H50	000646-31-1	87
4	2-methyloctacosane	408	C29H60	1000376-72-8	87
5	Octadecane	254	C18H38	000593-45-3	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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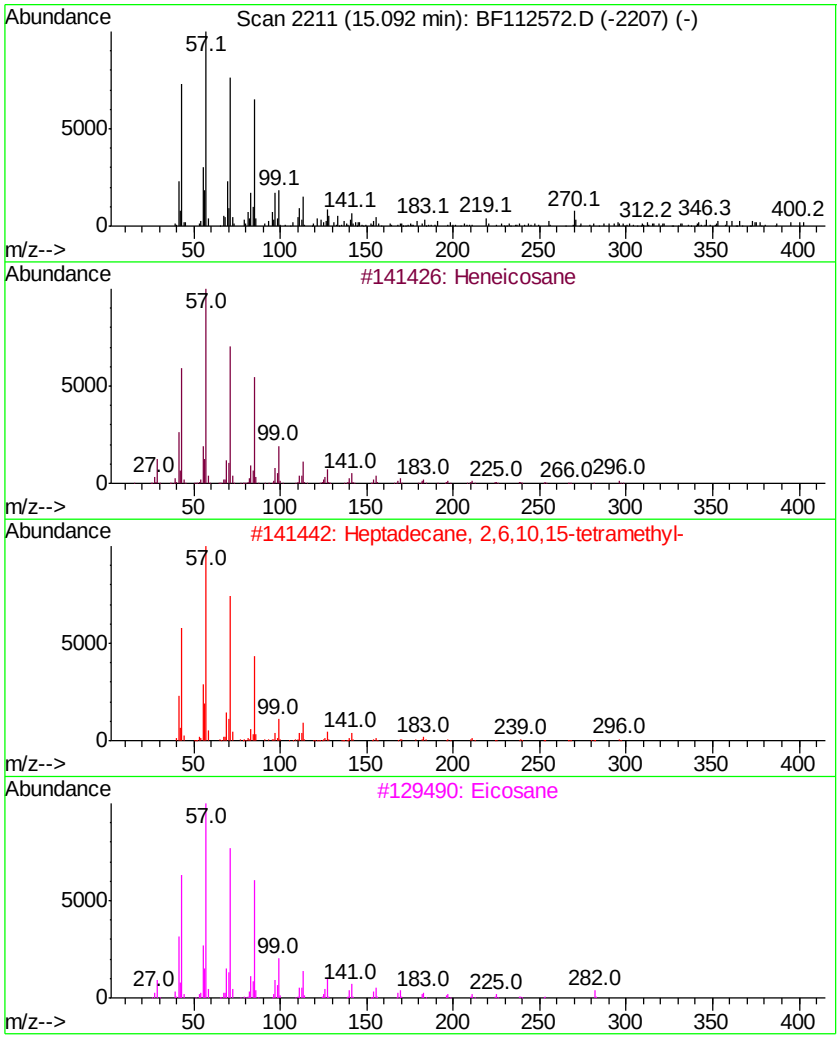
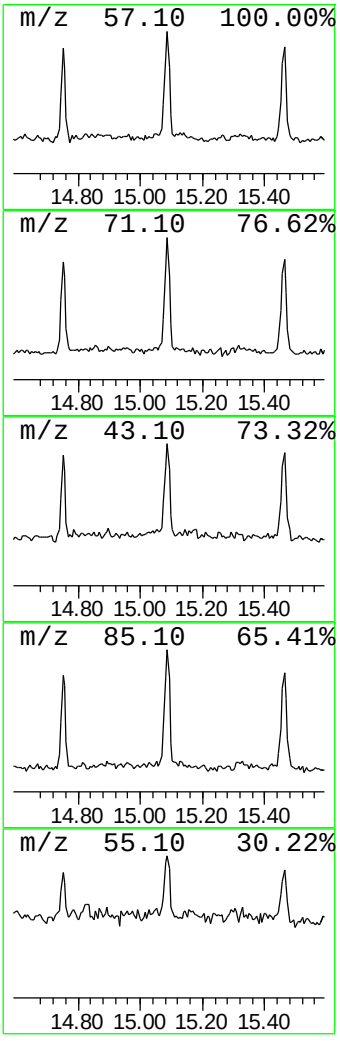
Peak Number 7 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.09	9.86 ng	249223	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	96
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91
3	Eicosane	282	C20H42	000112-95-8	91
4	2-methylhexacosane	380	C27H56	1000376-72-7	87
5	Hexadecane, 3-methyl-	240	C17H36	006418-43-5	87





Tentatively Identified Compound (LSC) summary

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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	32.2	ng	935779	1	6.83	581818	20.0
n-Hexadecanoic acid	11.87	3.3	ng	133331	4	11.36	810608	20.0
Cycloeicosane	13.83	3.3	ng	118095	5	14.01	712033	20.0
Eicosane	14.45	2.9	ng	102680	5	14.01	712033	20.0
Octacosane	14.75	5.6	ng	141034	6	15.49	505387	20.0
Heneicosane	15.09	9.9	ng	249223	6	15.49	505387	20.0