LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051823\
Data File : BF133448.D
Acq On : 18 May 2023 20:14
Operator : CG\JU
Sample : 02826-01 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-3-051723

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-BF042123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133448.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.646	261	265	270	rVB3	12657	20626	1.06%	0.104%
2	4.881	471	475	489	rVB	402354	440626	22.71%	2.214%
3	5.322	546	550	561	rBV	1843380	1770697	91.27%	8.896%
4	5.716	614	617	622	rVB	38610	33141	1.71%	0.166%
5	6.357	722	726	744	rBV	1895941	1768869	91.17%	8.887%
6	6.710	783	786	790	rBV	1383157	1215728	62.66%	6.108%
7	7.275	878	882	892	rBV	1271607	1076981	55.51%	5.411%
8	7.998	1001	1005	1008	rBV	1892420	1508275	77.74%	7.577%
9	9.069	1184	1187	1191	rBV	2155485	1940145	100.00%	9.747%
10	9.157	1198	1202	1207	rVB6	17077	21224	1.09%	0.107%
11	9.610	1277	1279	1283	rVB	40158	33331	1.72%	0.167%
12	9.751	1299	1303	1306	rBV	1725148	1458354	75.17%	7.327%
13	9.857	1317	1321	1325	rVB6	12471	22203	1.14%	0.112%
14	10.292	1393	1395	1402	rVB	20318	27998	1.44%	0.141%
15	10.457	1420	1423	1427	rBV	98661	92165	4.75%	0.463%
16	10.539	1433	1437	1448	rBV	880814	901293	46.45%	4.528%
17	10.663	1455	1458	1462	rVB4	25733	39395	2.03%	0.198%
18	11.139	1535	1539	1542	rVB2	24589	34991	1.80%	0.176%
19	11.192	1542	1548	1551	rBV8	10474	24039	1.24%	0.121%
20	11.233	1551	1555	1557	rVV	1539449	1301531	67.08%	6.539%
21	11.257	1557	1559	1562	rVV	155895	133799	6.90%	0.672%
22	11.304	1565	1567	1570	rVB	35544	35430	1.83%	0.178%
23	11.733	1637	1640	1642	rBV2	26924	27970	1.44%	0.141%
24	11.769	1642	1646	1656	rVB3	89819	135003	6.96%	0.678%
25	11.845	1656	1659	1661	rBV2	42509	42944	2.21%	0.216%
26	12.163	1710	1713	1715	rBV3	19933	23319	1.20%	0.117%
27	12.210	1719	1721	1728	rVV8	17743	40637	2.09%	0.204%
28	12.286	1731	1734	1736	rBV	44910	45783	2.36%	0.230%
29	12.321	1736	1740	1745	rVV5	46282	92641	4.77%	0.465%
30	12.445	1758	1761	1764	rBV	205609	181145	9.34%	0.910%
31	12.674	1796	1800	1802	rBV	198950	190164	9.80%	0.955%
32	12.698	1802	1804	1808	rVV3	51903	53060	2.73%	0.267%
33	12.815	1821	1824	1828	rBV	1847491	1599380	82.44%	8.035%
34	13.057	1862	1865	1870	rBV3	86446	102115	5.26%	0.513%
35	13.104	1871	1873	1877	rBV3	42343	46683	2.41%	0.235%
36	13.398	1921	1923	1926	rBV2	95720	75932	3.91%	0.381%

LSC Area Percent Report

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Operator : CG\JU
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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SU-3-051723

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-BF042123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.727	1977	1979	1981	rBV	122463	88760	4.57%	0.446%
38	13.874	1999	2004	2006	rBV	1282217	1307125	67.37%	6.567%
39	13.898	2006	2008	2011	rVB	115009	93412	4.81%	0.469%
40	14.045	2030	2033	2035	rVB	145446	125662	6.48%	0.631%
41	14.351	2082	2085	2087	rBV	161813	153699	7.92%	0.772%
42	14.451	2097	2102	2105	rBV5	214268	472748	24.37%	2.375%
43	14.645	2133	2135	2138	rVB	164718	137140	7.07%	0.689%
44	15.298	2242	2246	2249	rBV	839171	968809	49.93%	4.867%

Sum of corrected areas: 19904972

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Instrument :
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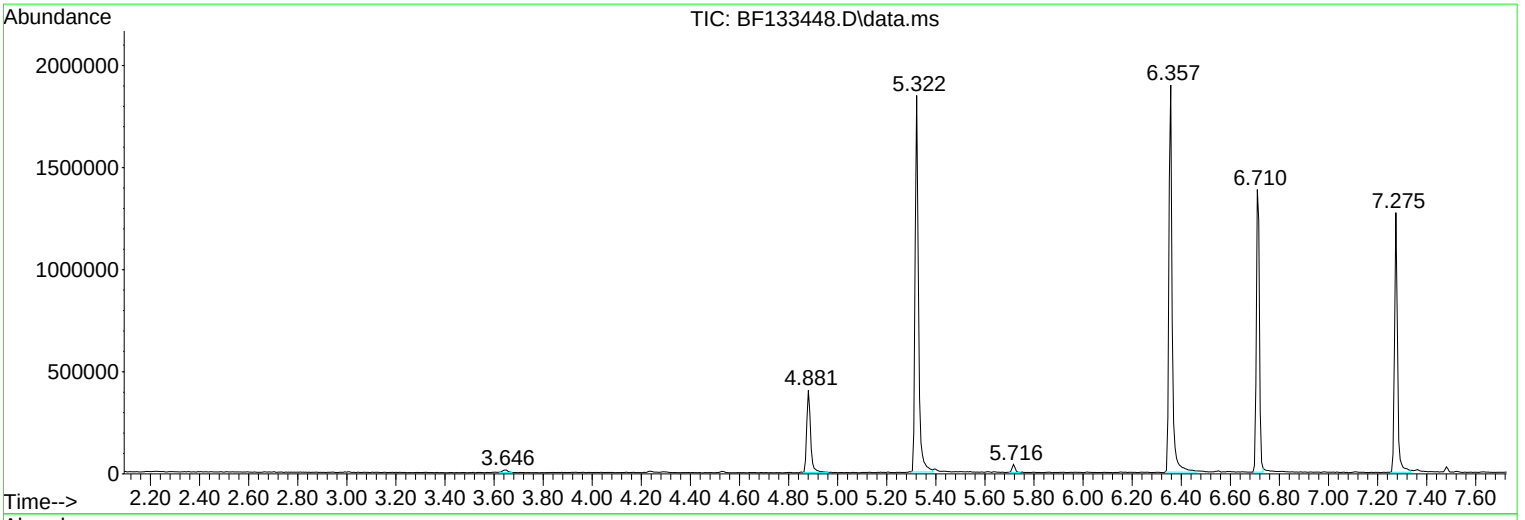
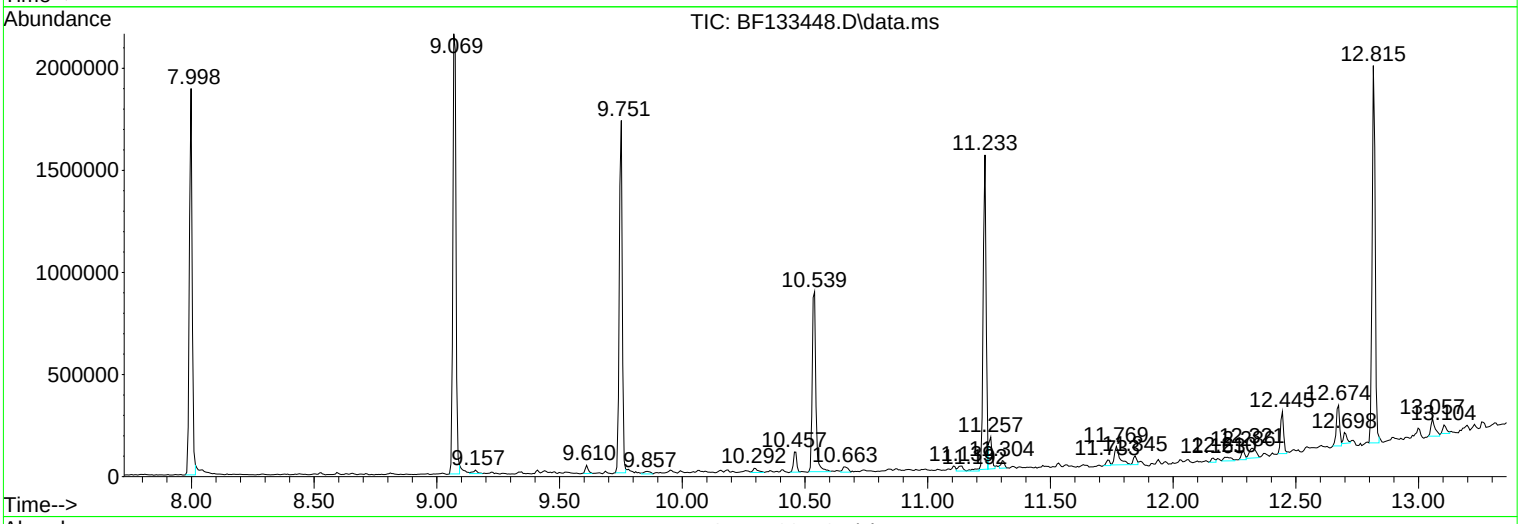
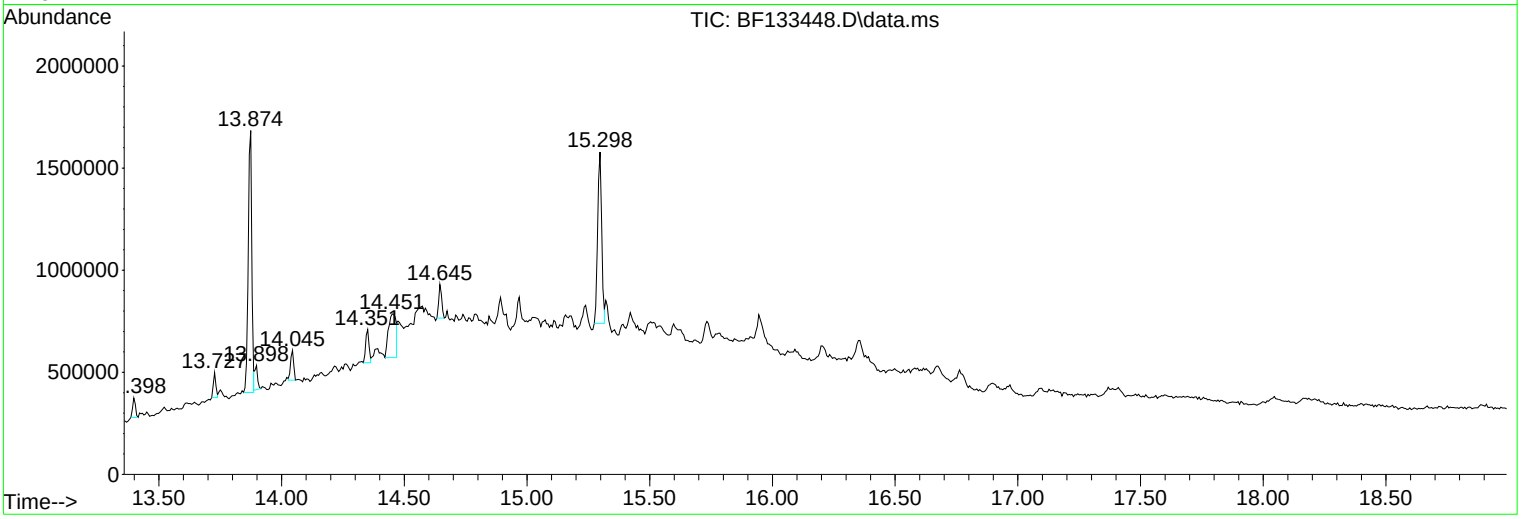
ClientSampleId :
SU-3-051723

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







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Data File : BF133448.D
Acq On : 18 May 2023 20:14
Operator : CG\JU
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Misc :
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Instrument :
BNA_F
ClientSampleId :
SU-3-051723

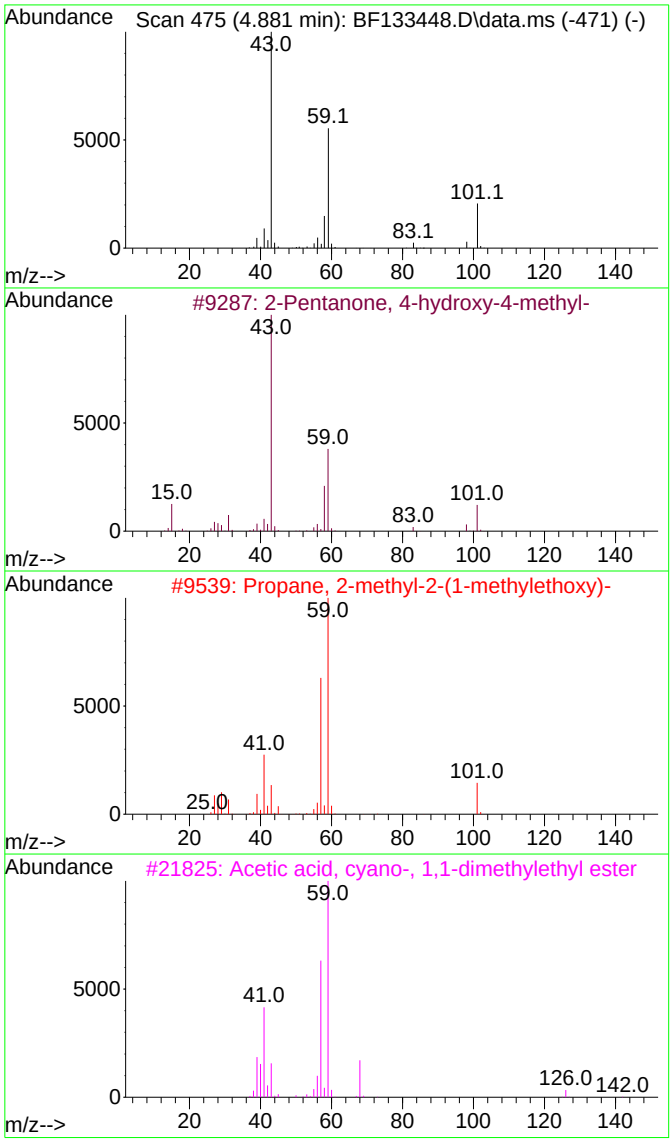
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

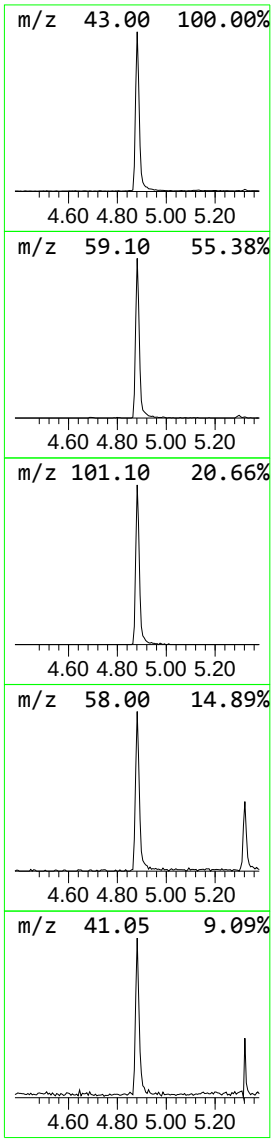
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.881	7.25 ng	440626	1,4-Dichlorobenzene-d4	6.710

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9





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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

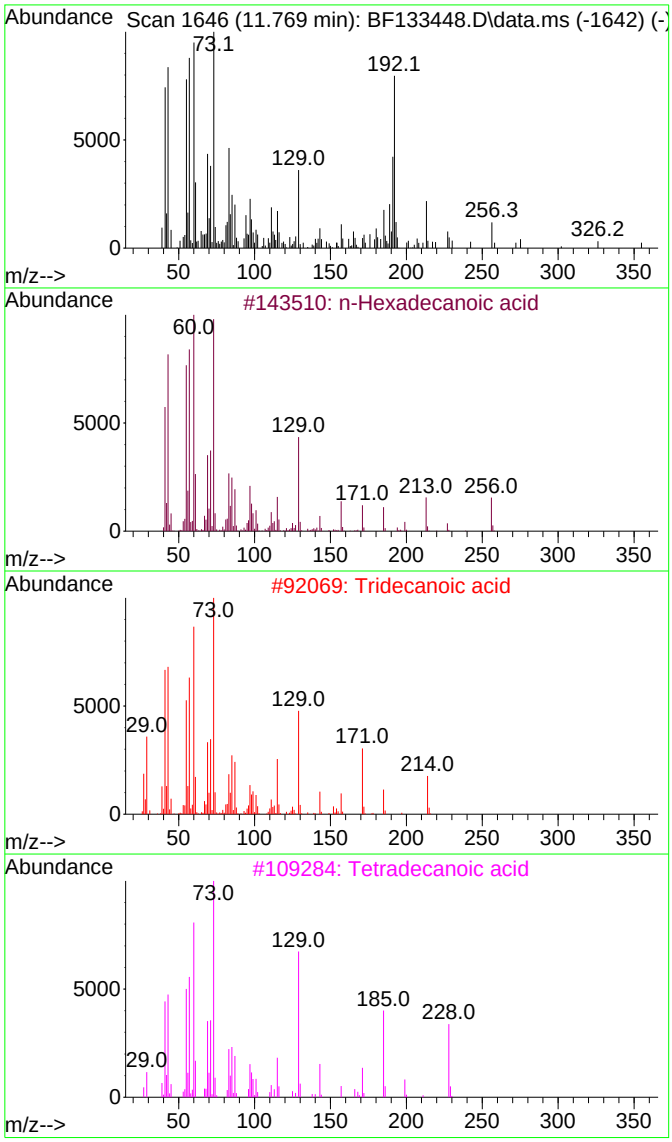
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

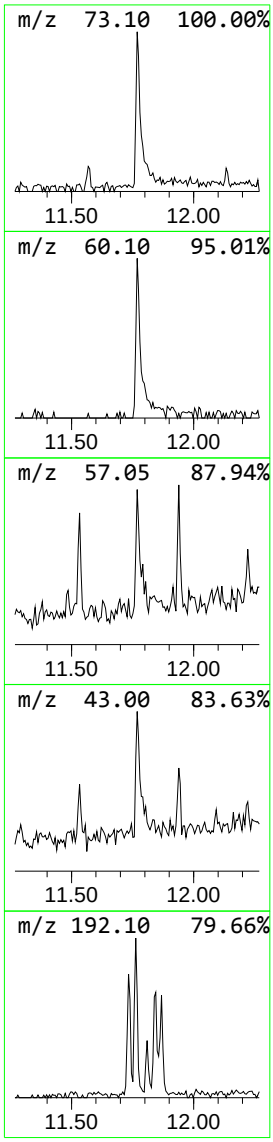
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.769	2.07 ng	135003	Phenanthrene-d10	11.233

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2	Tridecanoic acid	214	C13H26O2	000638-53-9	59
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	46
4	Undecanoic acid	186	C11H22O2	000112-37-8	38
5	Dodecanoic acid	200	C12H24O2	000143-07-7	38





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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SU-3-051723

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

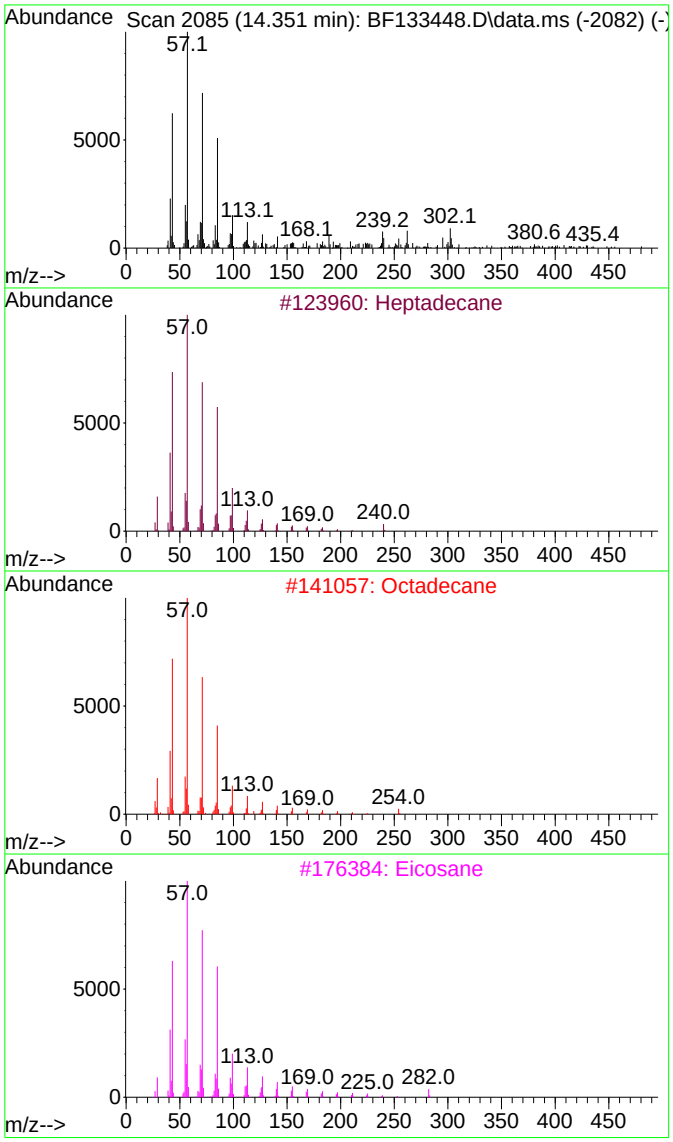
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

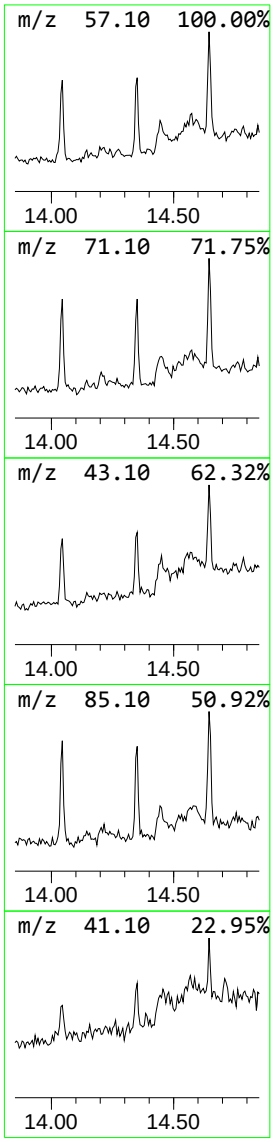
****

Peak Number 3 Heptadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.351	2.35 ng	153699	Chrysene-d12	13.874

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	93
2	Octadecane	254	C18H38	000593-45-3	92
3	Eicosane	282	C20H42	000112-95-8	86
4	Docosane	310	C22H46	000629-97-0	86
5	Pentadecane	212	C15H32	000629-62-9	86





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Misc :
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Instrument :
BNA_F
ClientSampleId :
SU-3-051723

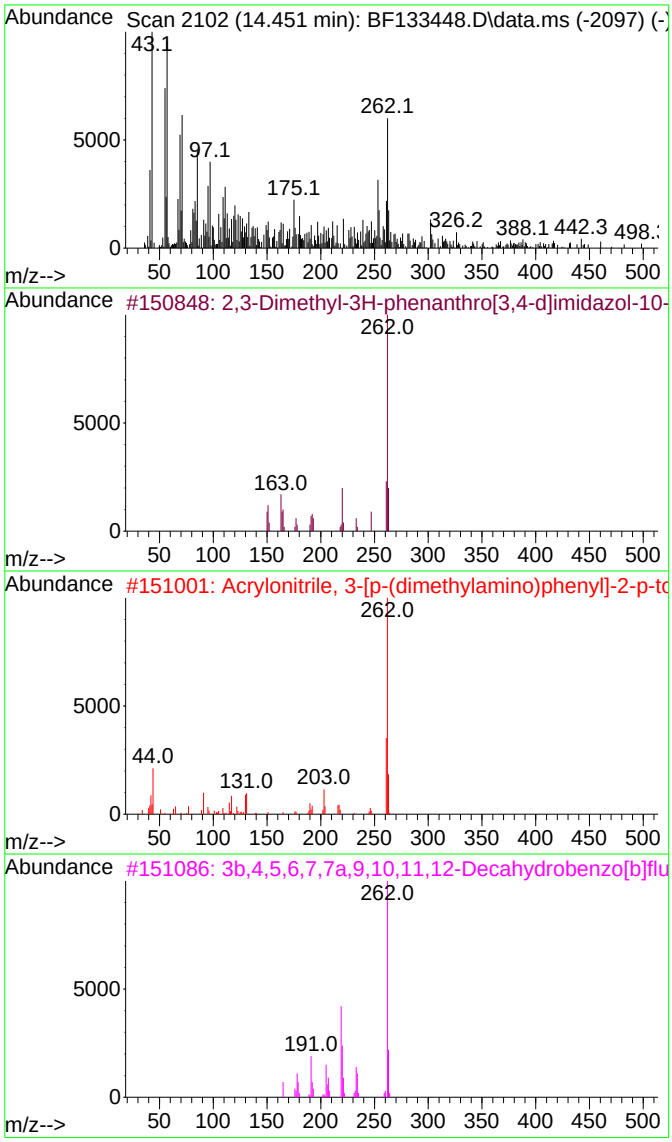
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

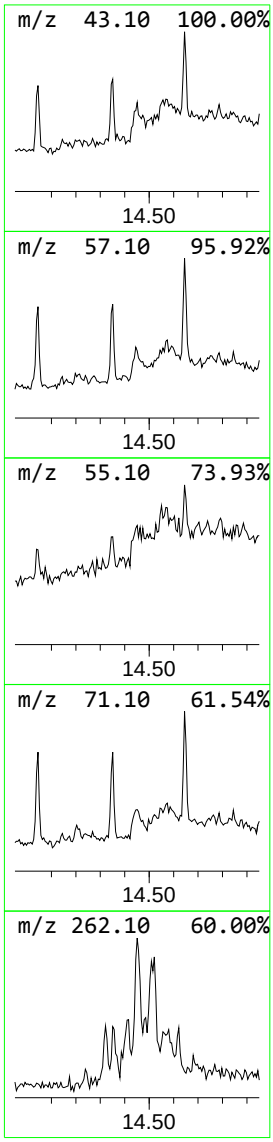
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2,3-Dimethyl-3H-phenanthro[... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.451	7.23 ng	472748	Chrysene-d12	13.874

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Dimethyl-3H-phenanthro[3,4-d...	262	C17H14N2O	098033-25-1	55
2	Acrylonitrile, 3-[p-(dimethylami...	262	C18H18N2	021994-54-7	38
3	3b,4,5,6,7,7a,9,10,11,12-Decahyd...	262	C20H22	1000080-20-7	38
4	Benzo[b]naphtho[2,3-d]thiophene,...	262	C18H14S	024964-16-7	35
5	Cyclohexane, 1-(1-tetradecylpent...	491	C35H70	055521-27-2	30





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

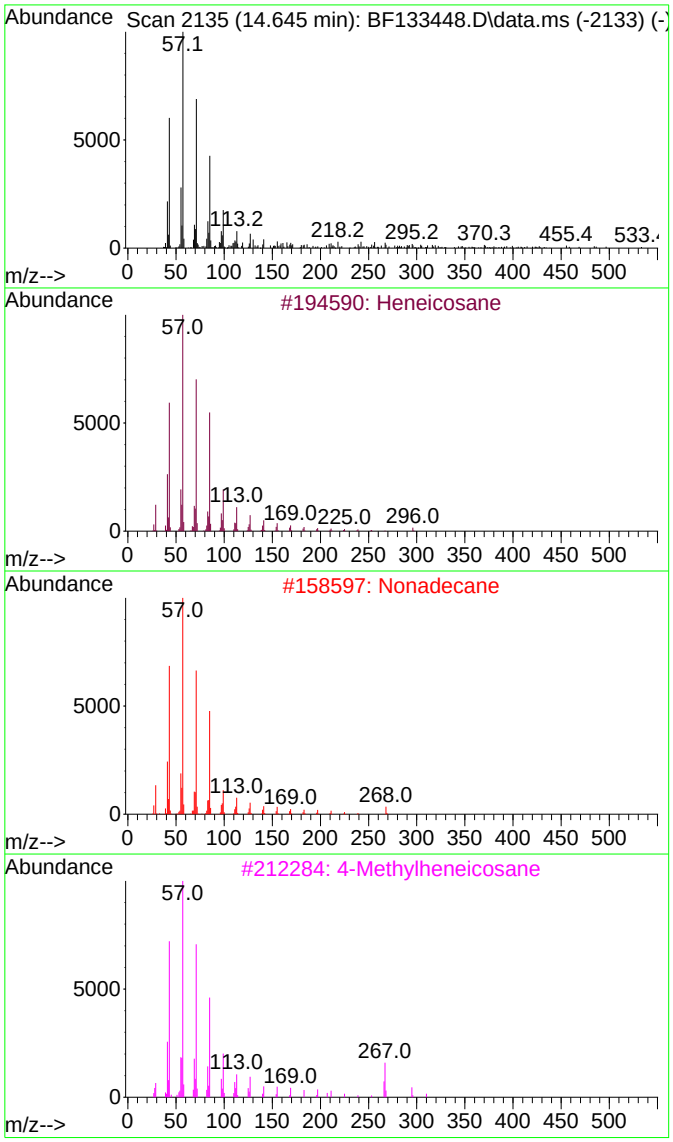
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

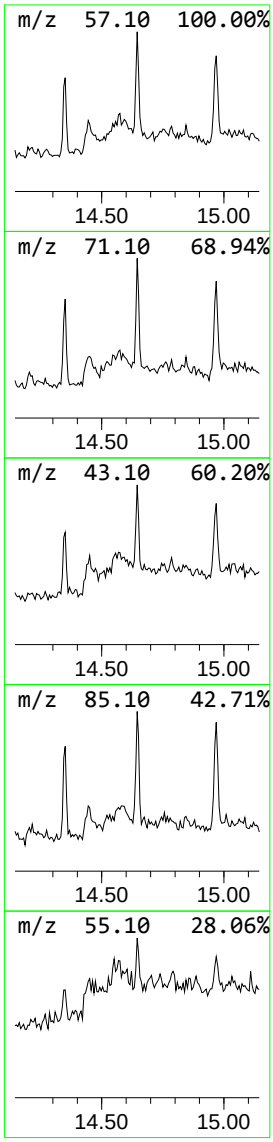
****

Peak Number 5 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.645	2.83 ng	137140	Perylene-d12	15.298

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	96
2	Nonadecane	268	C19H40	000629-92-5	91
3	4-Methylheneicosane	310	C22H46	025117-29-7	91
4	Heptadecane	240	C17H36	000629-78-7	91
5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	4.881	7.3	ng	440626	1	6.710	1215730	20.0
n-Hexadecanoic ...	11.769	2.1	ng	135003	4	11.233	1301530	20.0
Heptadecane	14.351	2.4	ng	153699	5	13.874	1307130	20.0
2,3-Dimethyl-3H...	14.451	7.2	ng	472748	5	13.874	1307130	20.0
Heneicosane	14.645	2.8	ng	137140	6	15.298	968809	20.0