LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050223\
Data File : BF133190.D
Acq On : 02 May 2023 15:48
Operator : CG\JU
Sample : 02568-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11938

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: BF133190.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.928	478	483	495	rVB	321792	420374	7.85%	0.896%
2	5.346	549	554	557	rBV	4836898	4761621	88.93%	10.147%
3	6.375	723	729	732	rBV	4580788	4838482	90.36%	10.310%
4	6.728	785	789	792	rBV	1622532	1226368	22.90%	2.613%
5	7.293	880	885	888	rBV	3324511	3168664	59.18%	6.752%
6	8.010	1003	1007	1011	rBV	1974904	1706057	31.86%	3.635%
7	9.092	1186	1191	1194	rBV	6063995	5354635	100.00%	11.410%
8	9.739	1298	1301	1303	rBV	233366	250534	4.68%	0.534%
9	9.763	1303	1305	1308	rVV	2356335	1874070	35.00%	3.993%
10	9.798	1308	1311	1315	rVB	100847	97753	1.83%	0.208%
11	10.310	1395	1398	1400	rBV	88103	74101	1.38%	0.158%
12	10.481	1423	1427	1430	rVB	1340306	1107351	20.68%	2.360%
13	10.557	1435	1440	1443	rBV	3405496	3282594	61.30%	6.995%
14	10.692	1458	1463	1468	rVB2	91291	127511	2.38%	0.272%
15	10.781	1475	1478	1482	rVB	76083	73147	1.37%	0.156%
16	11.151	1537	1541	1545	rVB2	74302	125812	2.35%	0.268%
17	11.245	1553	1557	1559	rBV	2254675	1937191	36.18%	4.128%
18	11.269	1559	1561	1564	rVV	948152	695841	13.00%	1.483%
19	11.322	1567	1570	1573	rVB	139074	119353	2.23%	0.254%
20	11.745	1639	1642	1645	rBV	113776	116029	2.17%	0.247%
21	11.786	1645	1649	1653	rBV2	806477	750745	14.02%	1.600%
22	11.857	1658	1661	1663	rVV	203898	210721	3.94%	0.449%
23	11.880	1663	1665	1670	rVB	95000	80730	1.51%	0.172%
24	12.063	1694	1696	1703	rVB2	102625	95445	1.78%	0.203%
25	12.298	1733	1736	1739	rBV	77562	65753	1.23%	0.140%
26	12.380	1747	1750	1755	rVB3	62156	71430	1.33%	0.152%
27	12.457	1759	1763	1766	rBV	1234820	1042118	19.46%	2.221%
28	12.569	1780	1782	1787	rBV2	188592	155177	2.90%	0.331%
29	12.680	1795	1801	1805	rBV	915858	1001618	18.71%	2.134%
30	12.739	1809	1811	1815	rVB3	75367	81081	1.51%	0.173%
31	12.839	1823	1828	1831	rVV	5056838	5071088	94.70%	10.806%
32	12.904	1834	1839	1842	rBV2	63885	95204	1.78%	0.203%
33	13.016	1855	1858	1860	rVB	134719	132669	2.48%	0.283%
34	13.080	1865	1869	1872	rVV2	139296	141134	2.64%	0.301%
35	13.116	1872	1875	1878	rBV	93232	81578	1.52%	0.174%
36	13.416	1924	1926	1928	rBV	82372	61310	1.14%	0.131%

LSC Area Percent Report

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Operator : CG\JU
Sample : 02568-01
Misc :
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Instrument : BNA_F
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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	13.516	1940	1943	1948	rVB	61513	74395	1.39%	0.159%
38	13.598	1953	1957	1960	rBV	1026311	869838	16.24%	1.854%
39	13.627	1960	1962	1965	rVB2	73378	72366	1.35%	0.154%
40	13.745	1980	1982	1990	rBV4	159728	249100	4.65%	0.531%
41	13.880	2000	2005	2008	rBV2	1571852	1706553	31.87%	3.637%
42	13.904	2008	2009	2012	rVB	373359	225000	4.20%	0.479%
43	14.063	2033	2036	2039	rVB2	96924	83821	1.57%	0.179%
44	14.269	2066	2071	2074	rBV	61361	76957	1.44%	0.164%
45	14.363	2084	2087	2090	rBV3	108878	112418	2.10%	0.240%
46	14.521	2111	2114	2118	rVB	57200	66658	1.24%	0.142%
47	14.663	2136	2138	2141	rVB2	76917	60137	1.12%	0.128%
48	14.733	2147	2150	2156	rBV2	82315	114519	2.14%	0.244%
49	14.804	2159	2162	2165	rVB2	71420	69363	1.30%	0.148%
50	14.892	2174	2177	2180	rBV	235170	310230	5.79%	0.661%
51	14.921	2180	2182	2187	rVB2	145792	133499	2.49%	0.284%
52	14.986	2190	2193	2197	rVB2	134011	156789	2.93%	0.334%
53	15.180	2222	2226	2232	rVB	159107	187188	3.50%	0.399%
54	15.239	2232	2236	2242	rVB	209483	243704	4.55%	0.519%
55	15.298	2242	2246	2250	rBV	935426	1117339	20.87%	2.381%
56	15.757	2320	2324	2330	rBV2	90902	135940	2.54%	0.290%
57	16.668	2474	2479	2487	rVB2	109531	209851	3.92%	0.447%
58	17.086	2544	2550	2557	rVB2	85112	157205	2.94%	0.335%

Sum of corrected areas: 46928159

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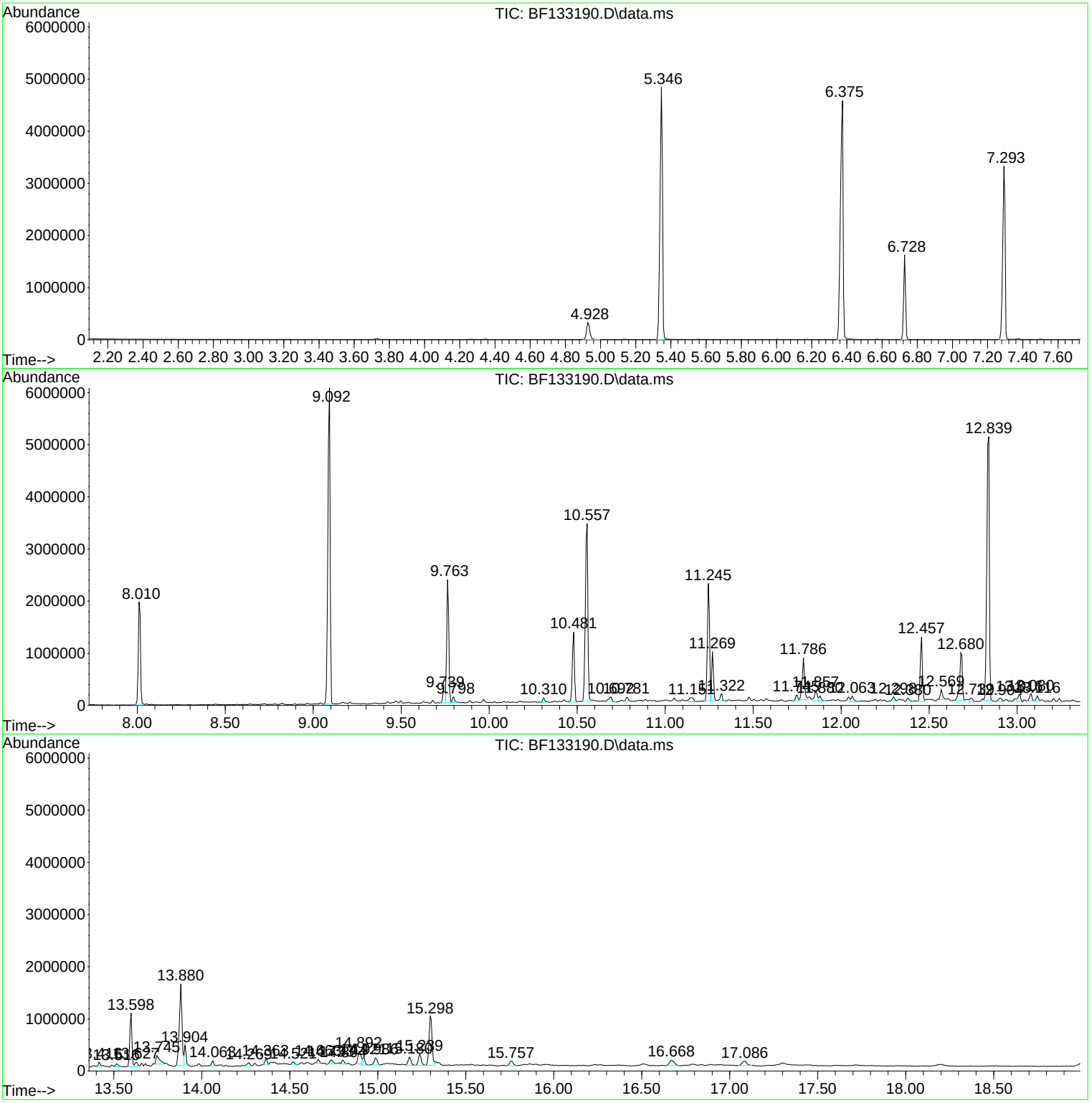
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11938

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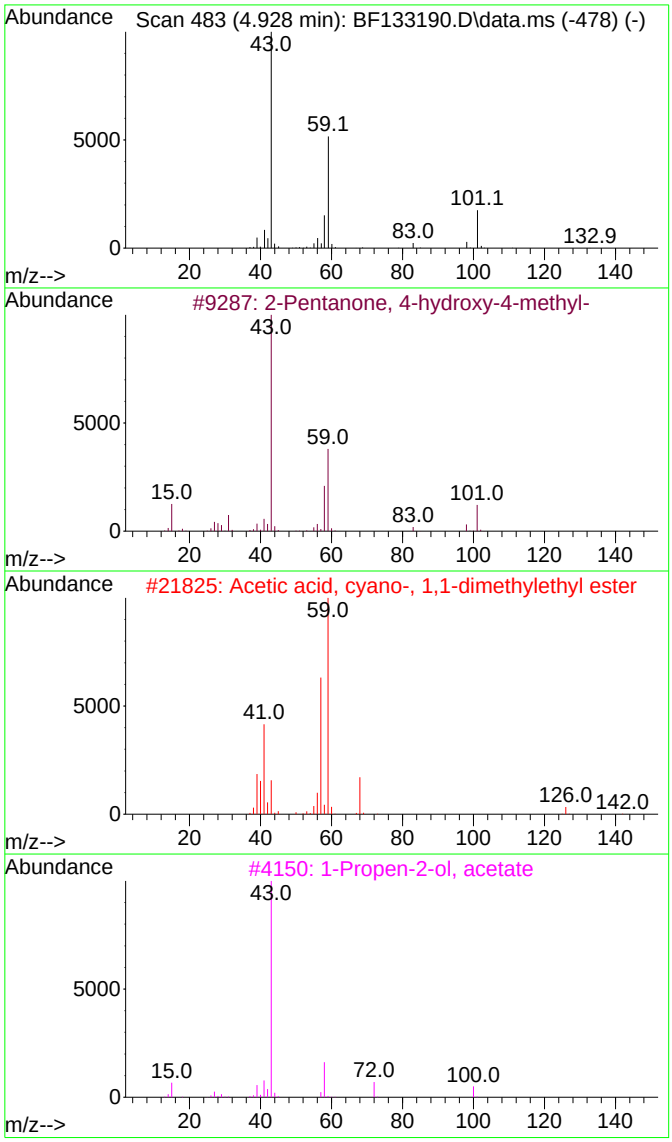
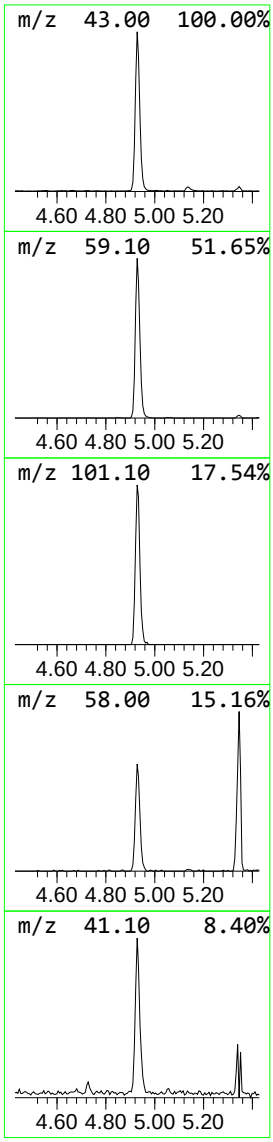
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.928	6.86 ng	420374	1,4-Dichlorobenzene-d4	6.728

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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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

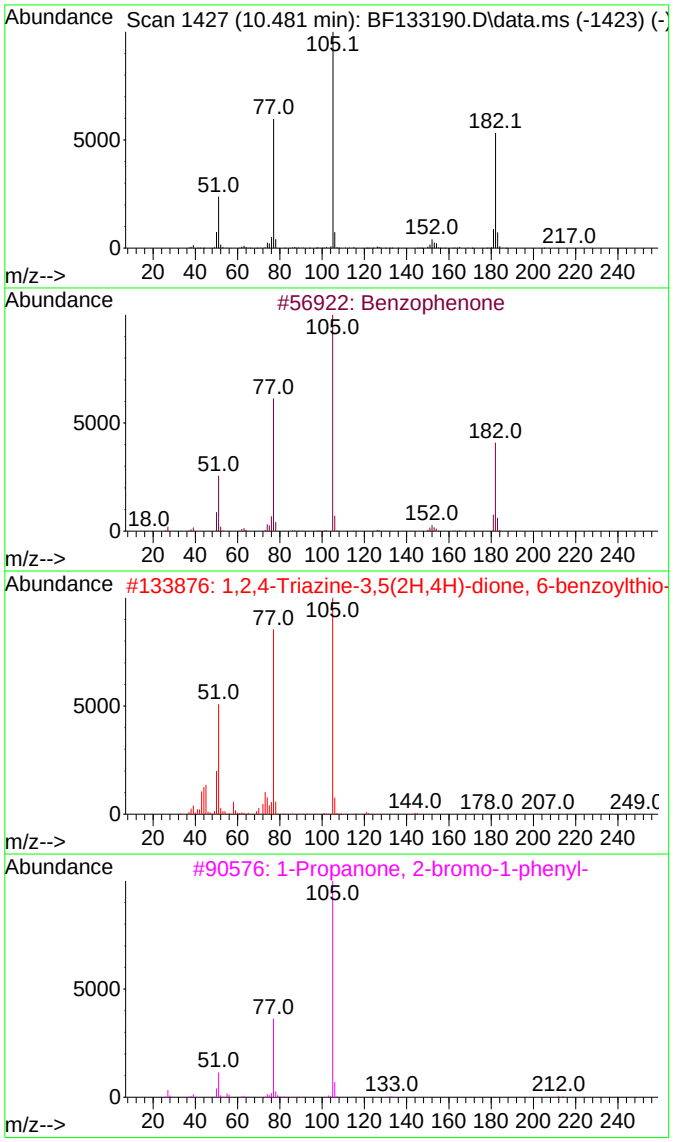
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

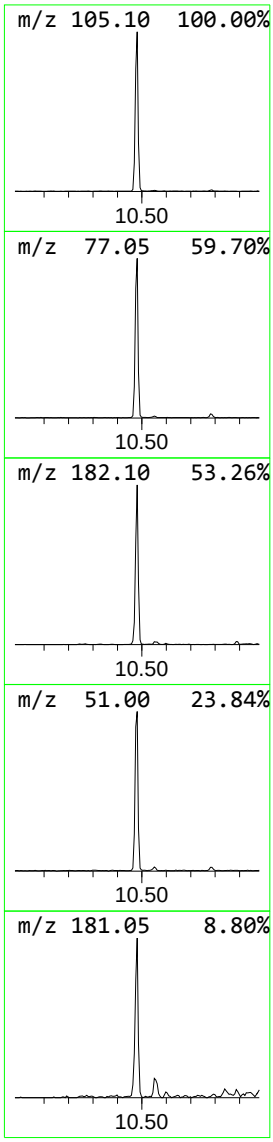
****

Peak Number 2 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.480	11.82 ng	1107350	Acenaphthene-d10	9.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	1,2,4-Triazine-3,5(2H,4H)-dione,...	249	C10H7N3O3S	024168-34-1	47
3	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
4	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	47
5	2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47





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TIC Library : C:\Database\NIST20.L
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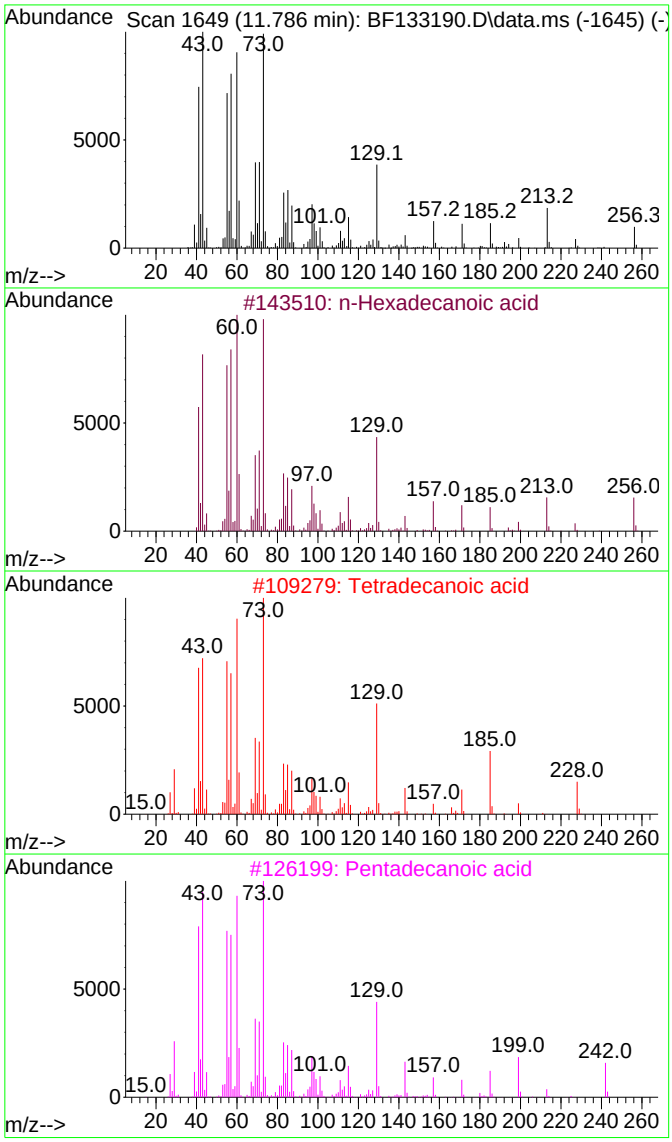
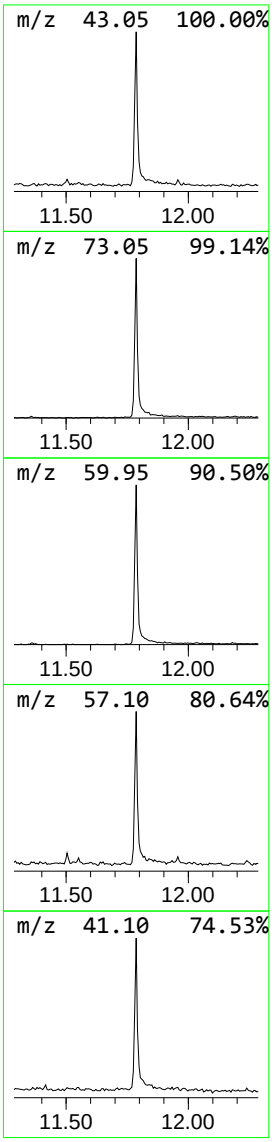
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.786	7.75 ng	750745	Phenanthrene-d10	11.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tridecanoic acid	214	C13H26O2	000638-53-9	90
5	n-Decanoic acid	172	C10H20O2	000334-48-5	81





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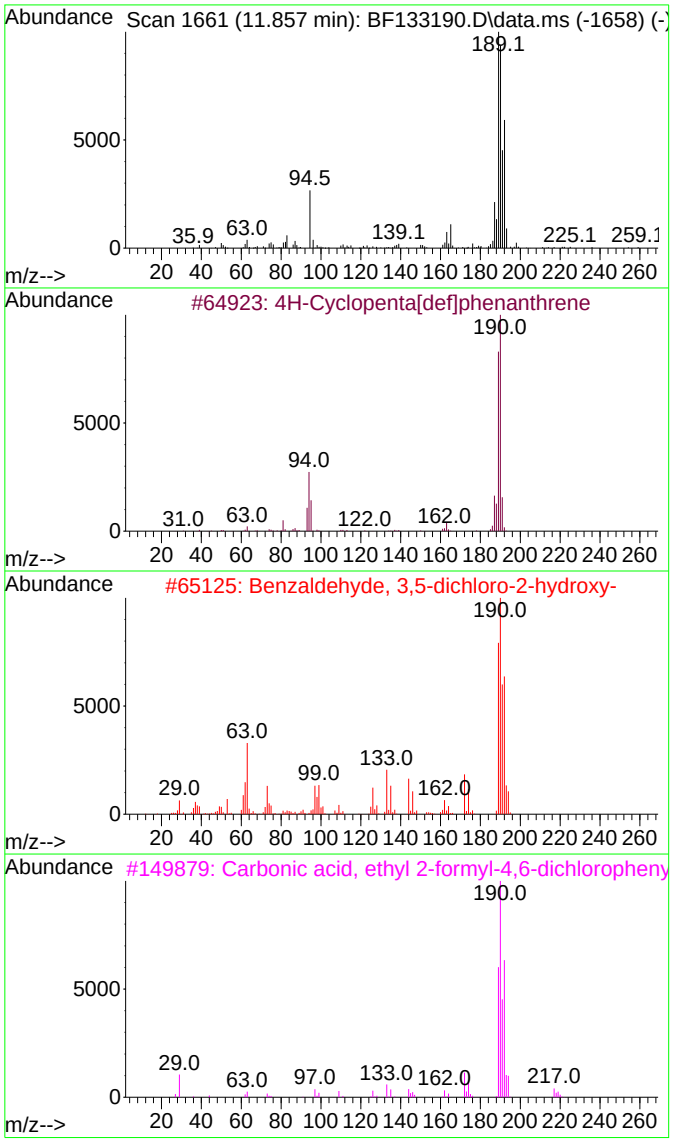
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

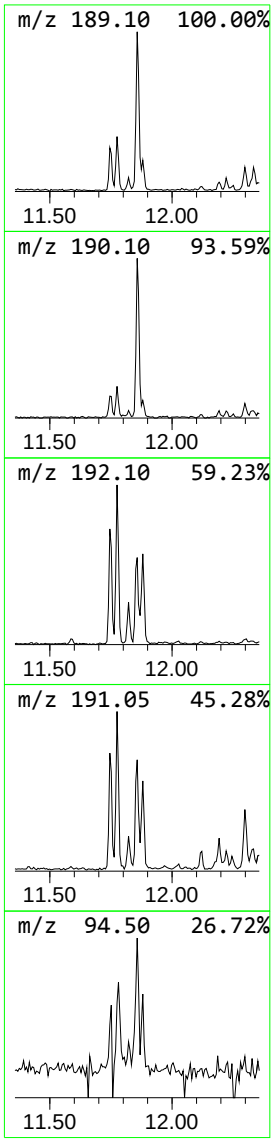
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	2.18 ng	210721	Phenanthrene-d10	11.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	50
3	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	50
4	Methyl diselenide	190	C2H6Se2	007101-31-7	38
5	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	30





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

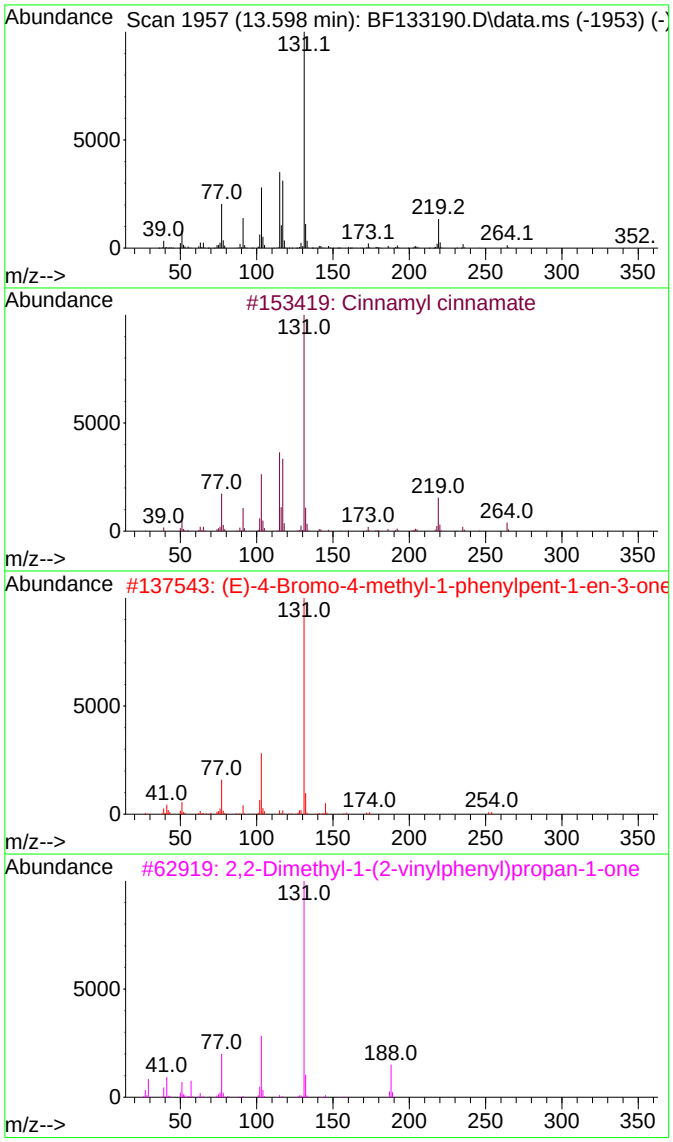
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

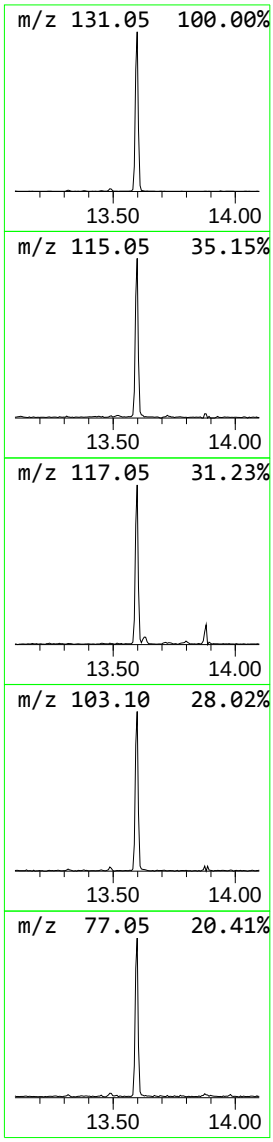
****

Peak Number 5 Cinnamyl cinnamate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.598	10.19 ng	869838	Chrysene-d12	13.880

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91
2	(E)-4-Bromo-4-methyl-1-phenylpen...	252	C12H13BrO	1000443-02-8	53
3	2,2-Dimethyl-1-(2-vinylphenyl)pr...	188	C13H16O	1000210-99-9	52
4	1,3-Phenylene, bis(3-phenylprope...	370	C24H18O4	1000259-62-4	50
5	2-Propenoic acid, 3-phenyl-, phe...	224	C15H12O2	025695-77-6	50





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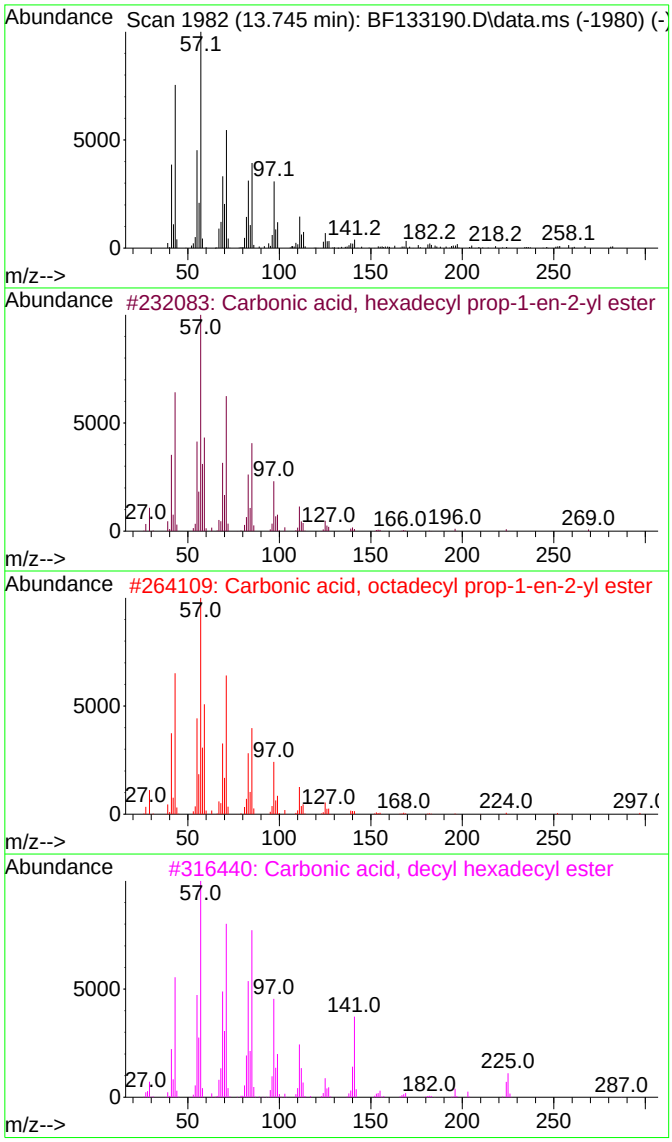
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

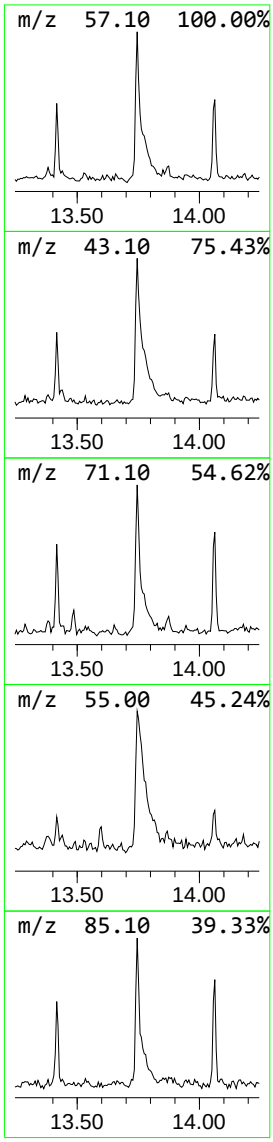
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Carbonic acid, hexadecyl pr... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.745	2.92 ng	249100	Chrysene-d12	13.880

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	91
2	Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	91
3	Carbonic acid, decyl hexadecyl e...	426	C27H54O3	1000383-16-5	87
4	Carbonic acid, octadecyl vinyl e...	340	C21H40O3	1000382-54-4	83
5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	83





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Instrument :
BNA_F
ClientSampleId :
72-11938

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

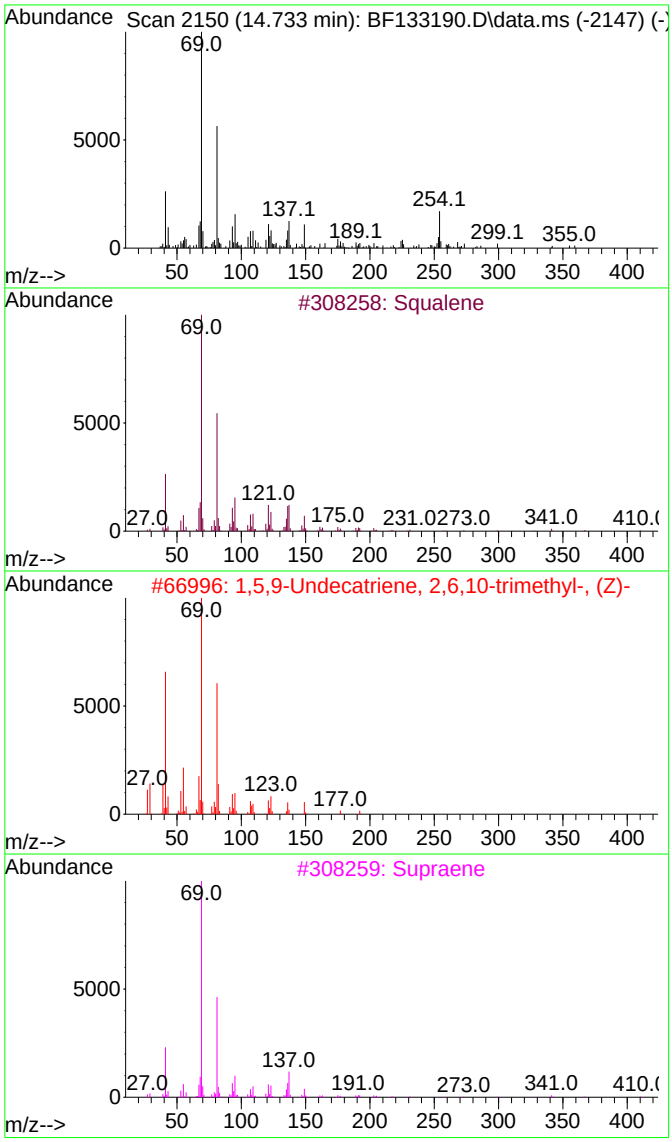
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

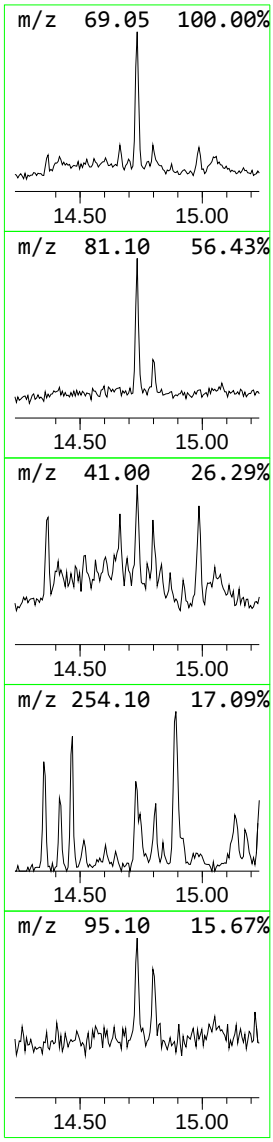
****

Peak Number 7 Squalene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.733	2.05 ng	114519	Perylene-d12	15.298

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	80
2	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	76
3	Supraene	410	C30H50	007683-64-9	74
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	62
5	1-(3,5-Dinitrophenoxy)-3,7,11-tr...	388	C21H28N2O5	1000187-44-2	53





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Misc :
ALS Vial : 13 Sample Multiplier: 1

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

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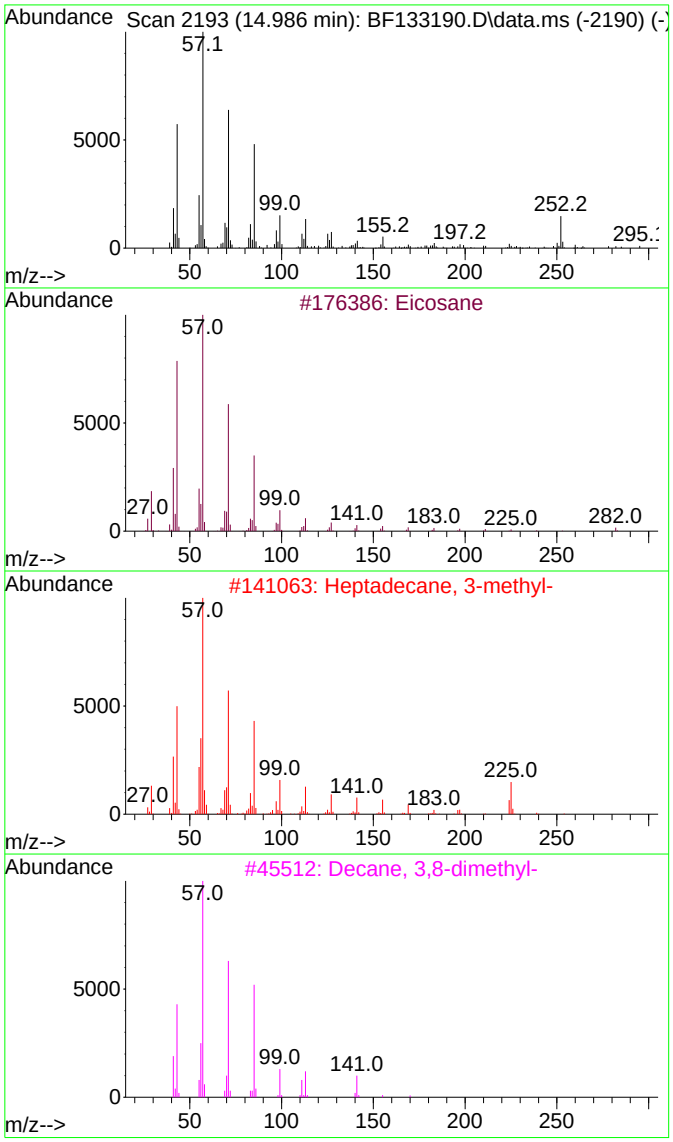
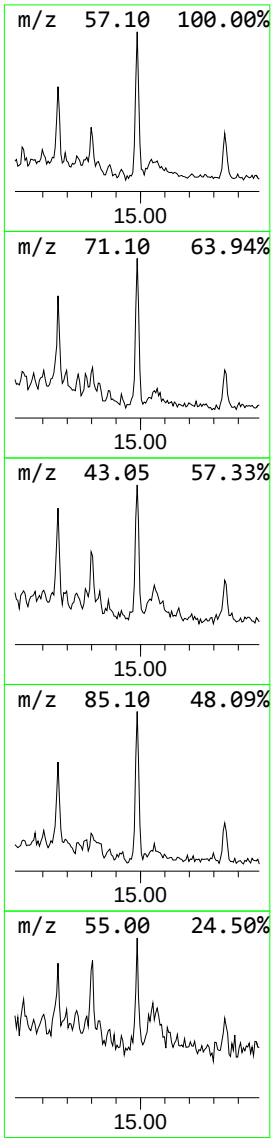
Peak Number 8 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.986	2.81 ng	156789	Perylene-d12	15.298

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Heptadecane, 3-methyl-	254	C18H38	006418-44-6	87
3	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	87
4	Heptadecane	240	C17H36	000629-78-7	83
5	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	83





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Data File : BF133190.D
Acq On : 02 May 2023 15:48
Operator : CG\JU
Sample : 02568-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11938

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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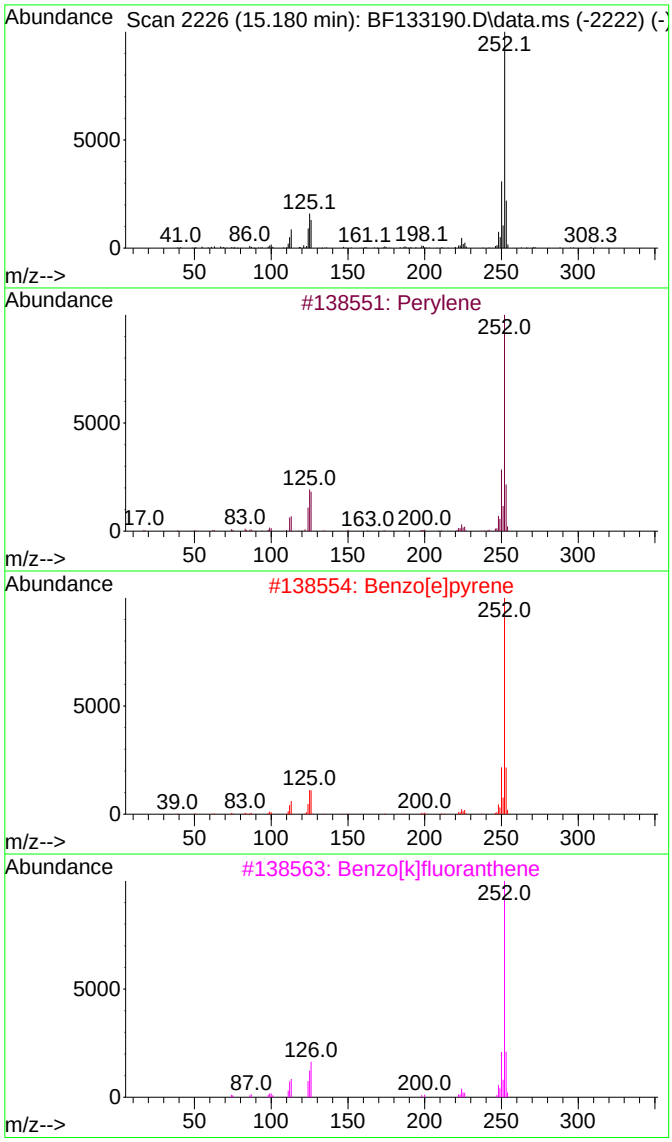
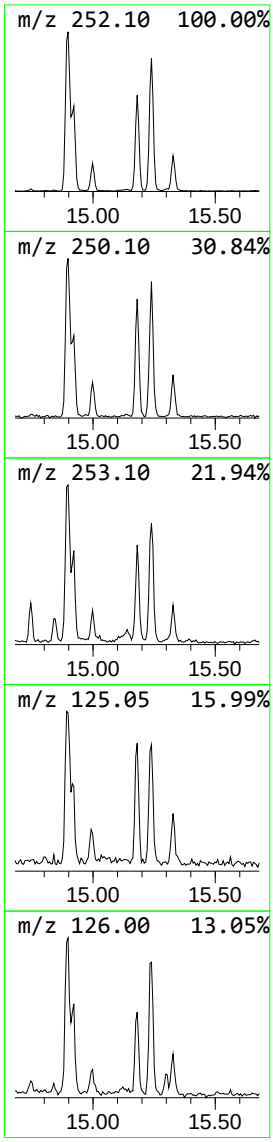
Peak Number 9 Perylene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.180	3.35 ng	187188	Perylene-d12	15.298

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	99
2	Benzo[e]pyrene	252	C20H12	000192-97-2	97
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
5	Benzo[a]pyrene	252	C20H12	000050-32-8	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050223\
Data File : BF133190.D
Acq On : 02 May 2023 15:48
Operator : CG\JU
Sample : 02568-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11938

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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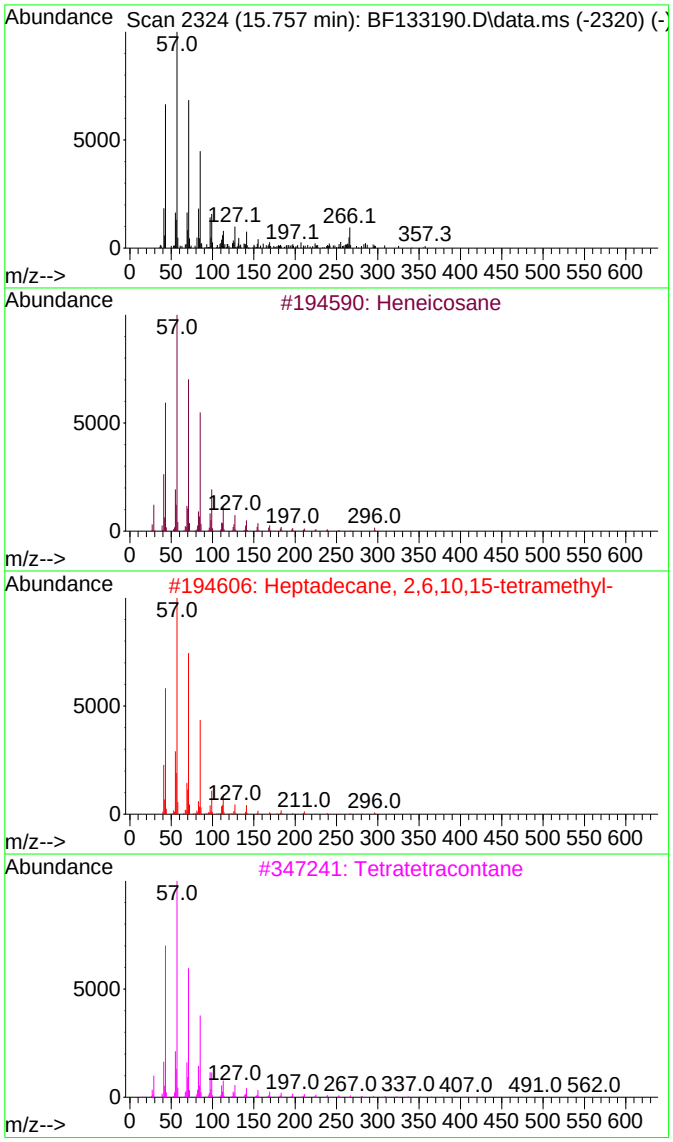
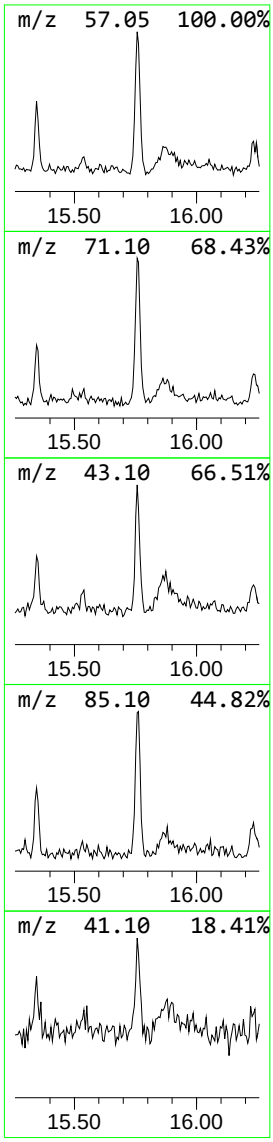
Peak Number 10 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.757	2.43 ng	135940	Perylene-d12	15.298

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	90
3	Tetratetracontane	619	C44H90	007098-22-8	83
4	Hexatriacontane	507	C36H74	000630-06-8	83
5	Behenyl chloride	344	C22H45Cl	042217-03-8	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050223\
Data File : BF133190.D
Acq On : 02 May 2023 15:48
Operator : CG\JU
Sample : 02568-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11938

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	4.928	6.9	ng	420374	1	6.728	1226370	20.0
Benzophenone	10.480	11.8	ng	1107350	3	9.763	1874070	20.0
n-Hexadecanoic ...	11.786	7.8	ng	750745	4	11.245	1937190	20.0
4H-Cyclopenta[d...	11.857	2.2	ng	210721	4	11.245	1937190	20.0
Cinnamyl cinnamate	13.598	10.2	ng	869838	5	13.880	1706550	20.0
Carbonic acid, ...	13.745	2.9	ng	249100	5	13.880	1706550	20.0
Squalene	14.733	2.0	ng	114519	6	15.298	1117340	20.0
Eicosane	14.986	2.8	ng	156789	6	15.298	1117340	20.0
Perylene	15.180	3.4	ng	187188	6	15.298	1117340	20.0
Heneicosane	15.757	2.4	ng	135940	6	15.298	1117340	20.0