LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011224\
Data File : BF137053.D
Acq On : 12 Jan 2024 17:26
Operator : CG\JU
Sample : P1118-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-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-BF122023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137053.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.158	8	12	24	rVB	12725	20144	1.76%	0.210%
2	3.363	215	217	221	rBV	8020	14424	1.26%	0.150%
3	5.016	495	498	507	rBV	70337	82300	7.17%	0.857%
4	5.428	565	568	592	rVB	949140	950335	82.83%	9.899%
5	6.434	735	739	756	rBV	1052636	951815	82.96%	9.915%
6	6.622	768	771	784	rBV	10200	20741	1.81%	0.216%
7	6.781	795	798	802	rBV	405260	331074	28.86%	3.449%
8	7.345	890	894	897	rBV	733652	602402	52.50%	6.275%
9	7.598	934	937	945	rBV	12235	13425	1.17%	0.140%
10	8.057	1012	1015	1023	rBV	498044	426240	37.15%	4.440%
11	8.381	1067	1070	1086	rBV3	14757	35667	3.11%	0.372%
12	9.134	1194	1198	1202	rBV	1314543	1147368	100.00%	11.952%
13	9.681	1284	1291	1295	rBV	11246	12844	1.12%	0.134%
14	9.816	1310	1314	1318	rBV	565135	445672	38.84%	4.642%
15	9.916	1326	1331	1343	rVB	362996	506080	44.11%	5.272%
16	10.610	1445	1449	1460	rBV	668421	609270	53.10%	6.347%
17	11.310	1564	1568	1570	rBV	497139	401349	34.98%	4.181%
18	11.333	1570	1572	1576	rVB	145157	110575	9.64%	1.152%
19	11.704	1631	1635	1637	rBV	19948	17942	1.56%	0.187%
20	11.816	1650	1654	1656	rBV	25442	22175	1.93%	0.231%
21	11.839	1656	1658	1665	rVV3	121116	115185	10.04%	1.200%
22	11.927	1670	1673	1675	rVV2	36558	37957	3.31%	0.395%
23	11.951	1675	1677	1681	rVB2	18383	16530	1.44%	0.172%
24	12.110	1702	1704	1707	rVB	15825	13112	1.14%	0.137%
25	12.145	1707	1710	1715	rVB	17831	16148	1.41%	0.168%
26	12.369	1743	1748	1750	rBV	18400	17972	1.57%	0.187%
27	12.410	1750	1755	1760	rVB5	36010	42840	3.73%	0.446%
28	12.527	1772	1775	1779	rBV	157916	147393	12.85%	1.535%
29	12.627	1789	1792	1798	rBV	15691	20708	1.80%	0.216%
30	12.763	1809	1815	1821	rBV	145181	154449	13.46%	1.609%
31	12.904	1835	1839	1842	rBV	1021798	844840	73.63%	8.800%
32	12.986	1848	1853	1857	rVB3	11586	18083	1.58%	0.188%
33	13.074	1863	1868	1869	rBV4	10494	14556	1.27%	0.152%
34	13.092	1869	1871	1874	rVB	19157	15848	1.38%	0.165%
35	13.198	1885	1889	1896	rVB2	19161	19134	1.67%	0.199%
36	13.610	1956	1959	1963	rVB	15493	14015	1.22%	0.146%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011224\
Data File : BF137053.D
Acq On : 12 Jan 2024 17:26
Operator : CG\JU
Sample : P1118-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-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-BF122023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.716	1972	1977	1980	rBV	19173	24345	2.12%	0.254%
38	13.821	1992	1995	1997	rVB2	15285	12487	1.09%	0.130%
39	13.869	1997	2003	2005	rBV6	16452	29734	2.59%	0.310%
40	13.968	2015	2020	2023	rBV2	376551	397186	34.62%	4.137%
41	13.992	2023	2024	2031	rVB	84575	66116	5.76%	0.689%
42	14.068	2031	2037	2040	rBV3	8112	15126	1.32%	0.158%
43	14.127	2044	2047	2054	rBV6	14462	19799	1.73%	0.206%
44	14.363	2082	2087	2090	rBV	17702	21489	1.87%	0.224%
45	14.721	2146	2148	2155	rVB3	18206	26750	2.33%	0.279%
46	14.816	2161	2164	2169	rVB	18123	17491	1.52%	0.182%
47	15.021	2195	2199	2207	rBV2	64057	124415	10.84%	1.296%
48	15.133	2215	2218	2221	rBV	11593	13030	1.14%	0.136%
49	15.327	2248	2251	2256	rVB	42502	52770	4.60%	0.550%
50	15.392	2258	2262	2267	rBV	56818	74481	6.49%	0.776%
51	15.457	2268	2273	2278	rBV	288731	376904	32.85%	3.926%
52	15.921	2348	2352	2356	rVB6	11007	16126	1.41%	0.168%
53	16.980	2526	2532	2537	rBV3	24050	48590	4.23%	0.506%
54	17.433	2606	2609	2617	rVB2	15895	32533	2.84%	0.339%

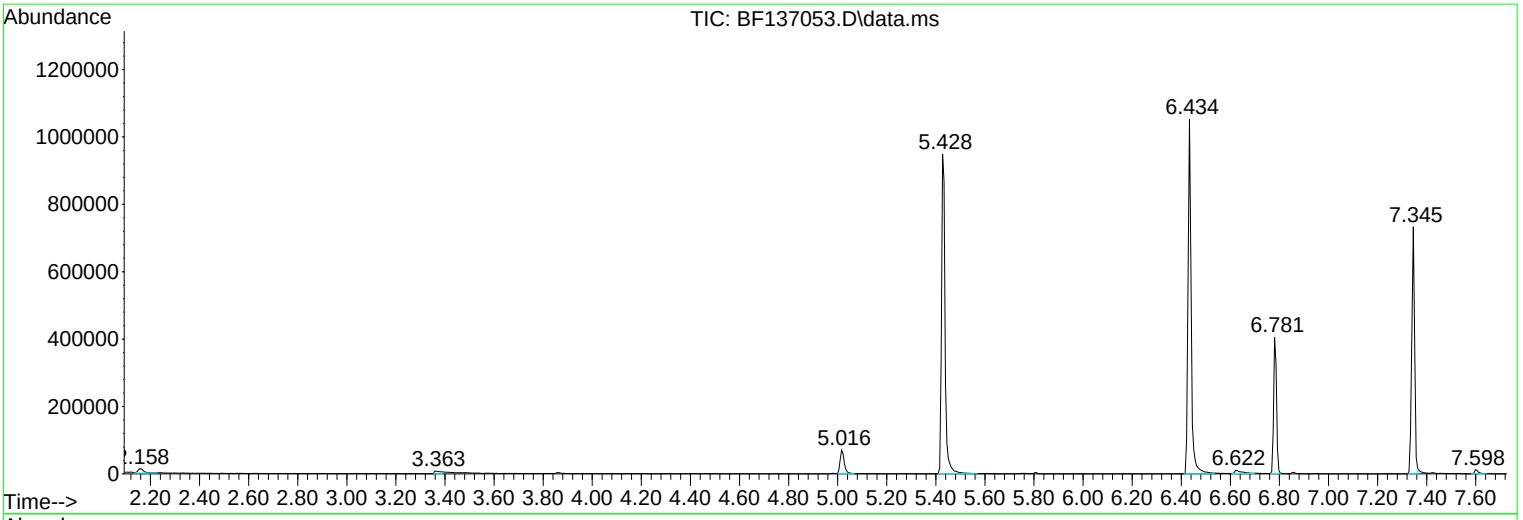
Sum of corrected areas: 9599984

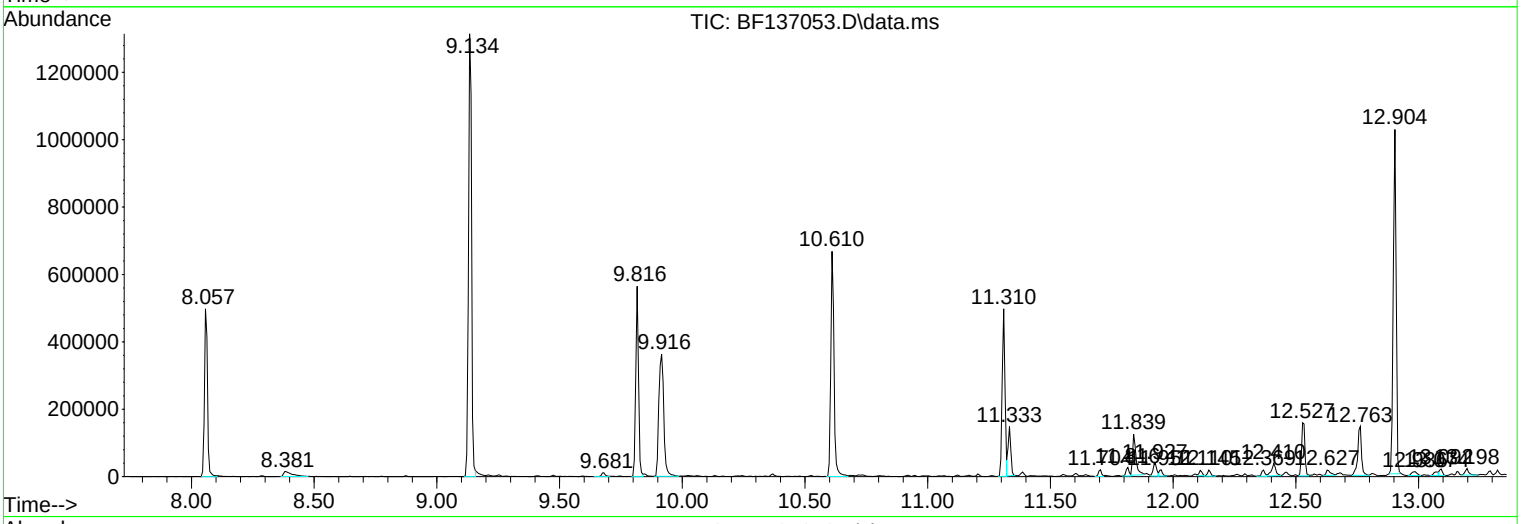
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011224\
Data File : BF137053.D
Acq On : 12 Jan 2024 17:26
Operator : CG\JU
Sample : P1118-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

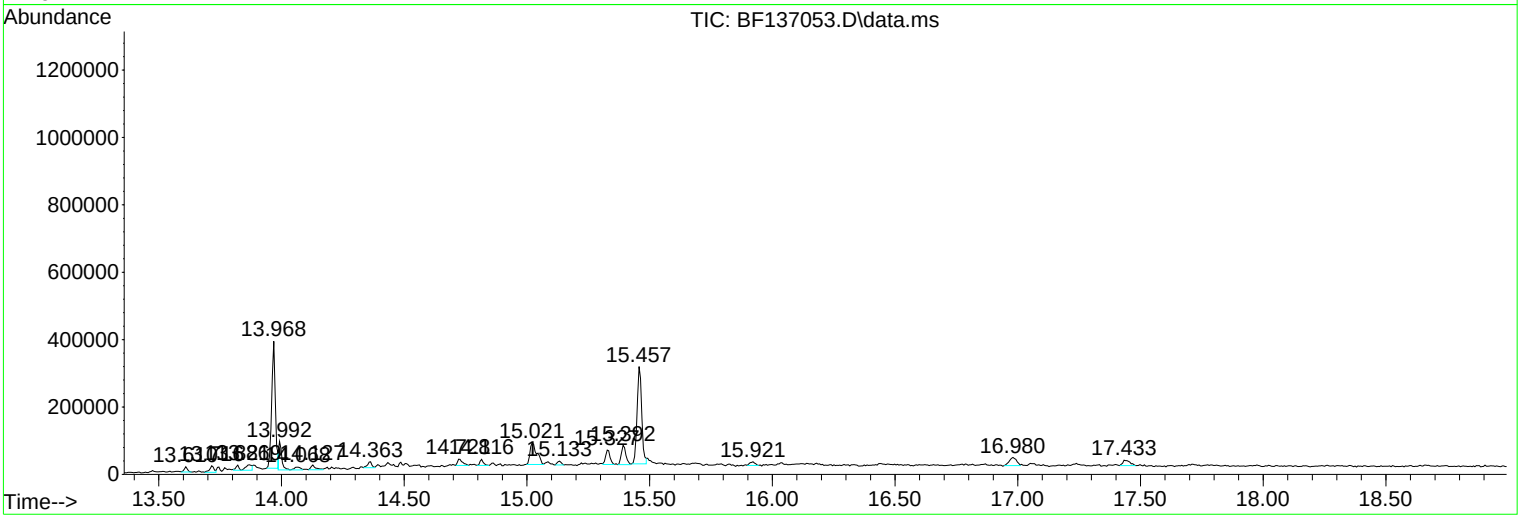
Instrument :
BNA_F
ClientSampleId :
WC-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011224\
Data File : BF137053.D
Acq On : 12 Jan 2024 17:26
Operator : CG\JU
Sample : P1118-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2

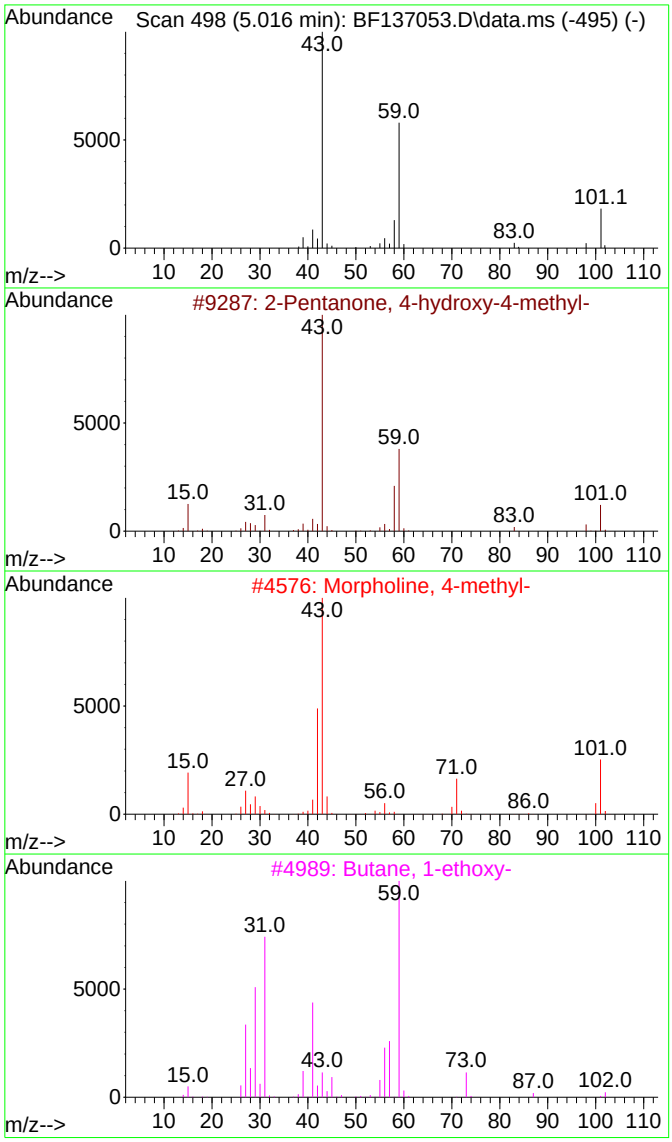
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

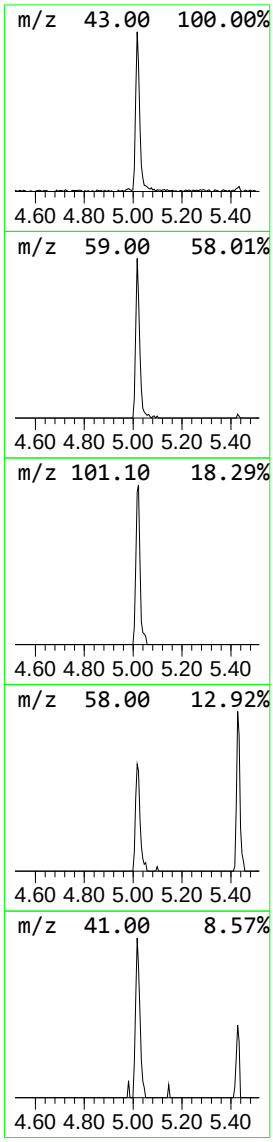
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.016	4.97 ng	82300	1,4-Dichlorobenzene-d4	6.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011224\
Data File : BF137053.D
Acq On : 12 Jan 2024 17:26
Operator : CG\JU
Sample : P1118-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

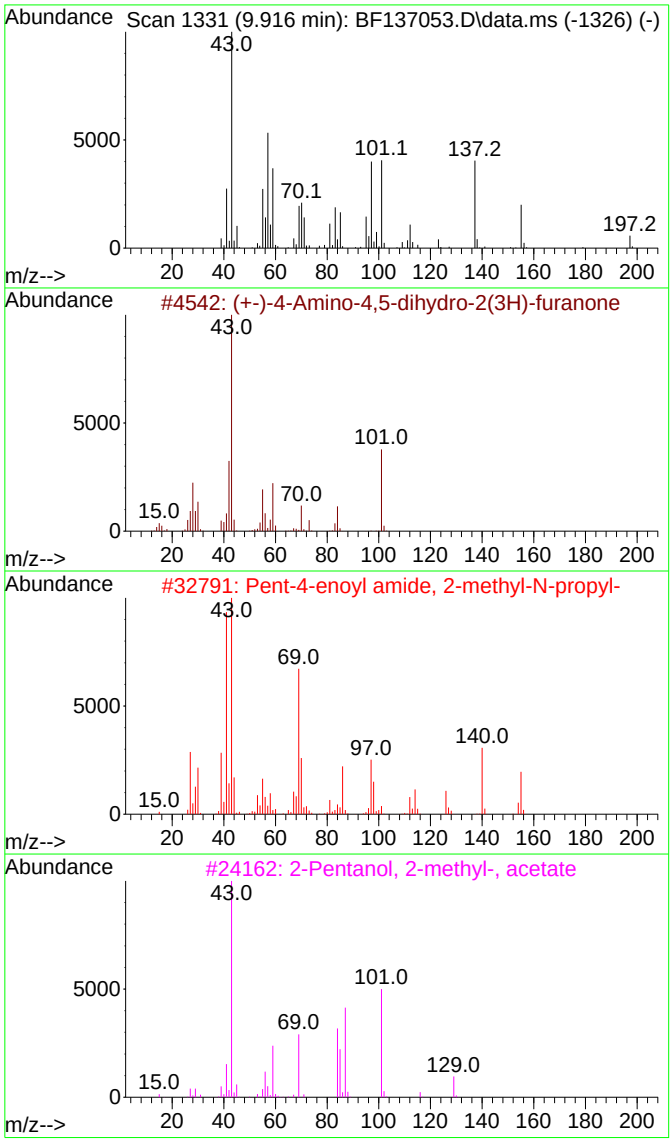
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

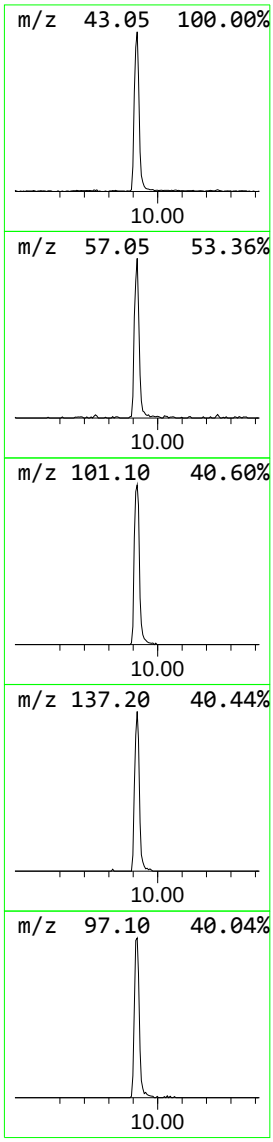
****

Peak Number 2 unknown9.916 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.916	22.71 ng	506080	Acenaphthene-d10	9.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	22
2	Pent-4-enoyl amide, 2-methyl-N-p...	155	C9H17NO	1000420-35-2	14
3	2-Pentanol, 2-methyl-, acetate	144	C8H16O2	034859-98-8	10
4	2-t-Butyl-5-propyl-[1,3]dioxolan...	186	C10H18O3	157733-17-0	10
5	Pentanoic acid, 4,4-dimethyl-3-o...	158	C8H14O3	055107-14-7	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011224\
Data File : BF137053.D
Acq On : 12 Jan 2024 17:26
Operator : CG\JU
Sample : P1118-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

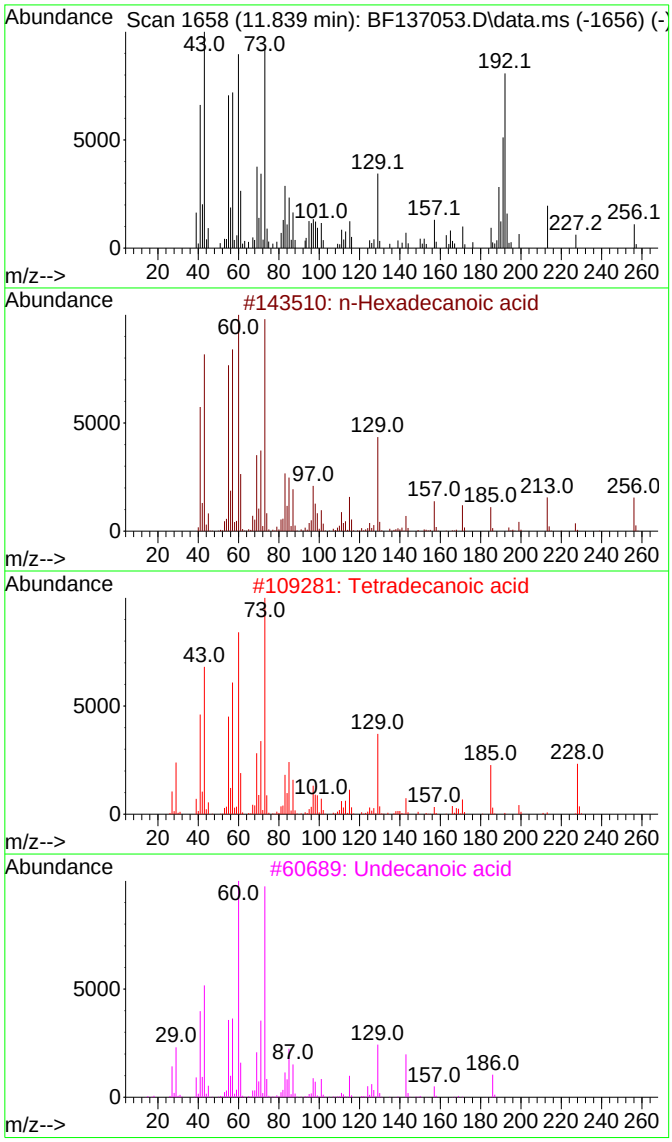
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

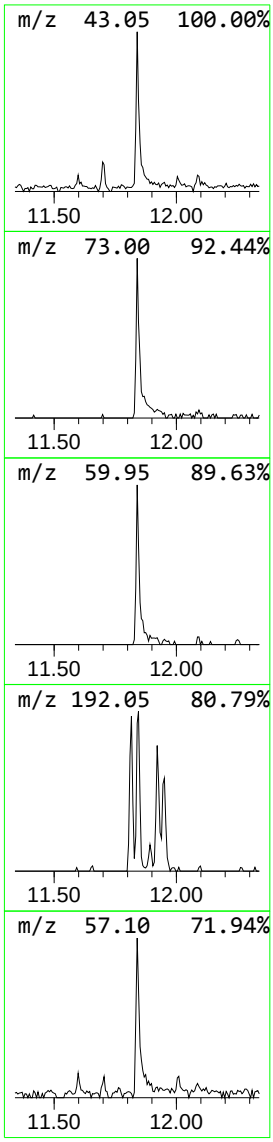
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	5.74 ng	115185	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	46
3	Undecanoic acid	186	C11H22O2	000112-37-8	46
4	n-Decanoic acid	172	C10H20O2	000334-48-5	42
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	41





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011224\
Data File : BF137053.D
Acq On : 12 Jan 2024 17:26
Operator : CG\JU
Sample : P1118-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2

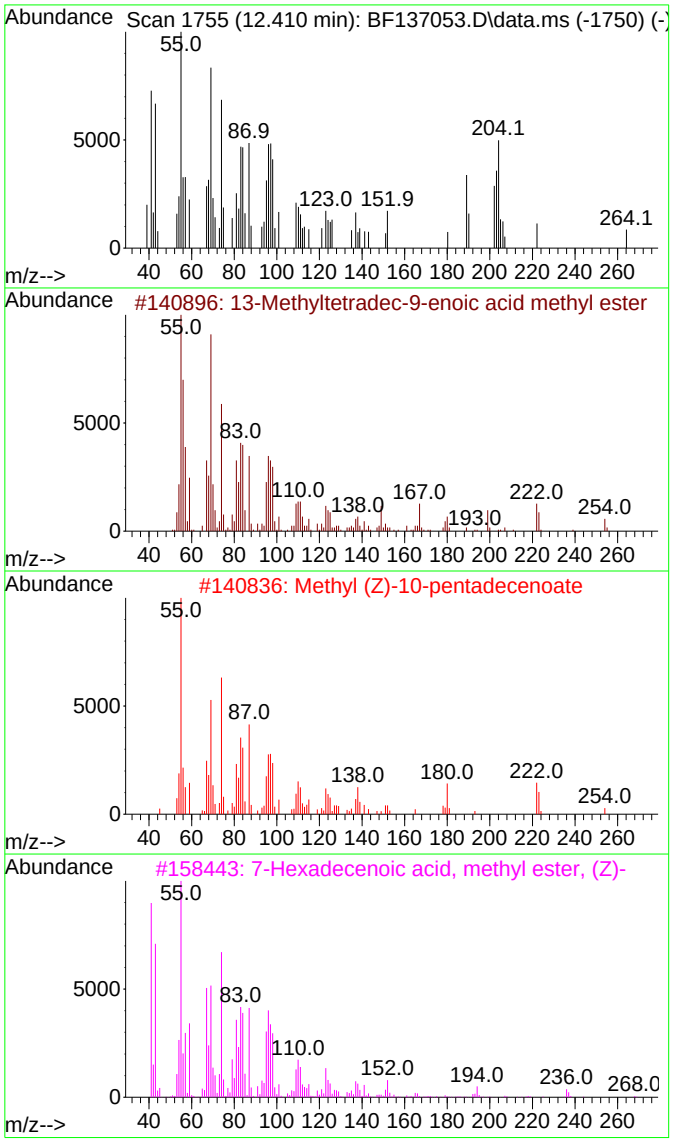
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

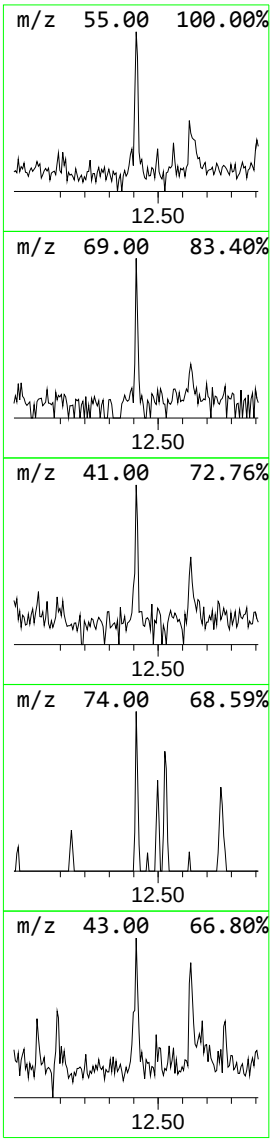
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 13-Methyltetradec-9-enoic a... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.410	2.13 ng	42840	Phenanthrene-d10	11.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Methyltetradec-9-enoic acid m...	254	C16H30O2	1010365-89-8	68
2	Methyl (Z)-10-pentadecenoate	254	C16H30O2	1000426-92-2	46
3	7-Hexadecenoic acid, methyl este...	268	C17H32O2	056875-67-3	46
4	Cyclopropaneoctanoic acid, 2-hex...	282	C18H34O2	010152-61-1	43
5	9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011224\
Data File : BF137053.D
Acq On : 12 Jan 2024 17:26
Operator : CG\JU
Sample : P1118-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

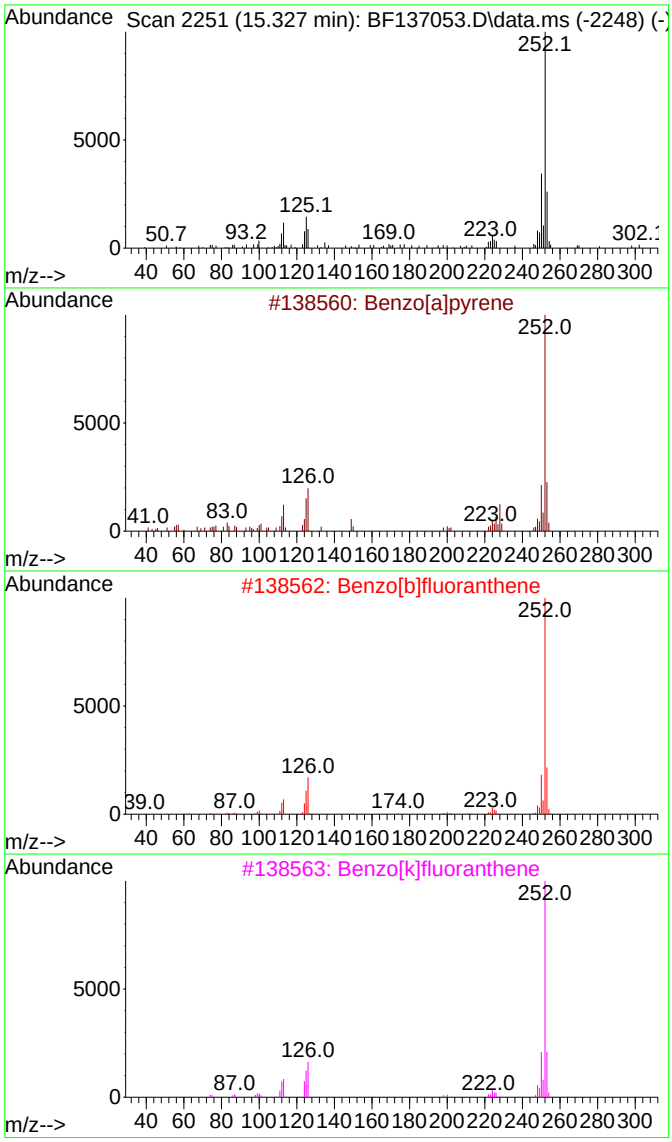
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

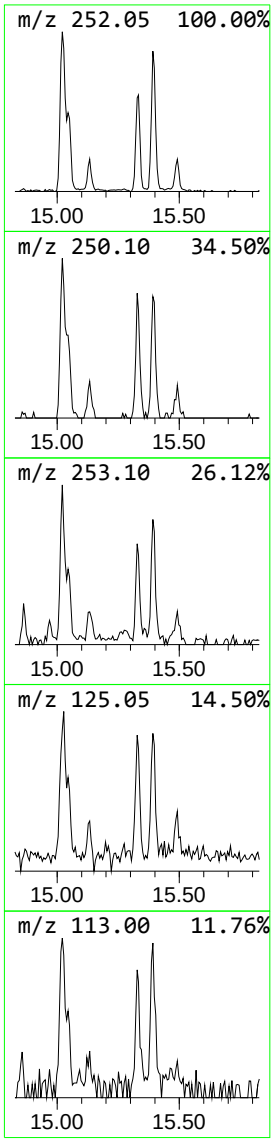
****

Peak Number 5 Perylene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.327	2.80 ng	52770	Perylene-d12	15.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[a]pyrene	252	C20H12	000050-32-8	93
2	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
4	Perylene	252	C20H12	000198-55-0	90
5	Benzo[e]pyrene	252	C20H12	000192-97-2	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011224\
Data File : BF137053.D
Acq On : 12 Jan 2024 17:26
Operator : CG\JU
Sample : P1118-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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-...	5.016	5.0	ng	82300	1	6.781	331074	20.0
unknown9.916	9.916	22.7	ng	506080	3	9.816	445672	20.0
n-Hexadecanoic ...	11.839	5.7	ng	115185	4	11.310	401349	20.0
13-Methyltetrad...	12.410	2.1	ng	42840	4	11.310	401349	20.0
Perylene	15.327	2.8	ng	52770	6	15.457	376904	20.0