LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030724\
Data File : BF137536.D
Acq On : 07 Mar 2024 18:19
Operator : CG\JU
Sample : P1688-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-5

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-BF022924.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137536.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	12	18	33	rVB	1269164	1739192	41.84%	4.744%
2	5.534	582	586	608	rBV	3786236	3956905	95.20%	10.792%
3	6.516	749	753	779	rBV	3634293	4156277	100.00%	11.336%
4	6.875	811	814	832	rBV	1329005	1291659	31.08%	3.523%
5	7.434	905	909	923	rBV	2592373	2528676	60.84%	6.897%
6	8.151	1027	1031	1049	rBV	1721860	1714788	41.26%	4.677%
7	8.481	1083	1087	1096	rBV3	20067	47912	1.15%	0.131%
8	9.228	1210	1214	1217	rBV	4755554	3988636	95.97%	10.879%
9	9.904	1326	1329	1333	rBV	2087710	1815978	43.69%	4.953%
10	9.939	1333	1335	1342	rVV	73553	82410	1.98%	0.225%
11	10.010	1342	1347	1353	rVB	79915	105618	2.54%	0.288%
12	10.698	1460	1464	1478	rBV	2376057	2321909	55.87%	6.333%
13	11.398	1580	1583	1586	rBV	1737906	1671696	40.22%	4.560%
14	11.427	1586	1588	1593	rVV	529325	495310	11.92%	1.351%
15	11.480	1593	1597	1606	rVB	97715	128720	3.10%	0.351%
16	11.651	1620	1626	1633	rBV3	29441	59556	1.43%	0.162%
17	11.910	1666	1670	1672	rBV	70636	66524	1.60%	0.181%
18	11.945	1672	1676	1680	rVV2	138132	178289	4.29%	0.486%
19	12.022	1685	1689	1691	rVV2	100474	127927	3.08%	0.349%
20	12.039	1691	1692	1700	rVB	52465	57451	1.38%	0.157%
21	12.210	1714	1721	1724	rBV2	45768	61726	1.49%	0.168%
22	12.463	1760	1764	1767	rBV2	43303	52197	1.26%	0.142%
23	12.621	1787	1791	1797	rBV	697176	631887	15.20%	1.723%
24	12.851	1825	1830	1834	rBV	578193	601950	14.48%	1.642%
25	12.910	1837	1840	1844	rVB2	47276	55058	1.32%	0.150%
26	13.004	1852	1856	1864	rVB	3611862	3170406	76.28%	8.647%
27	13.074	1864	1868	1873	rVB3	38800	61238	1.47%	0.167%
28	13.186	1885	1887	1891	rVB	66160	61527	1.48%	0.168%
29	13.245	1893	1897	1901	rBV3	56637	80481	1.94%	0.220%
30	13.292	1901	1905	1908	rBV	61287	69114	1.66%	0.189%
31	13.592	1952	1956	1959	rBV	80907	78516	1.89%	0.214%
32	13.816	1989	1994	1996	rBV2	45674	63396	1.53%	0.173%
33	13.921	2008	2012	2020	rBV2	259846	343000	8.25%	0.936%
34	14.063	2029	2036	2039	rBV2	1314137	1462127	35.18%	3.988%
35	14.086	2039	2040	2050	rVB	259264	274339	6.60%	0.748%
36	14.245	2064	2067	2069	rVB	89652	75634	1.82%	0.206%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030724\
Data File : BF137536.D
Acq On : 07 Mar 2024 18:19
Operator : CG\JU
Sample : P1688-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-5

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-BF022924.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.551	2116	2119	2122	rBV2	130451	124289	2.99%	0.339%
38	14.880	2173	2175	2182	rVB2	69953	88116	2.12%	0.240%
39	14.963	2185	2189	2196	rBV3	63903	96009	2.31%	0.262%
40	15.145	2215	2220	2223	rBV	238580	370615	8.92%	1.011%
41	15.257	2235	2239	2244	rVB2	97183	118185	2.84%	0.322%
42	15.468	2271	2275	2282	rVB	141392	202735	4.88%	0.553%
43	15.533	2282	2286	2292	rBV	184835	252892	6.08%	0.690%
44	15.604	2292	2298	2303	rVV	951103	1275936	30.70%	3.480%
45	15.674	2307	2310	2316	rVB4	43910	62143	1.50%	0.169%
46	16.162	2389	2393	2400	rBV2	43322	71880	1.73%	0.196%
47	17.204	2565	2570	2580	rBV2	58069	144140	3.47%	0.393%
48	17.421	2602	2607	2613	rBV5	30388	67867	1.63%	0.185%
49	17.686	2647	2652	2664	rVB2	47354	110834	2.67%	0.302%

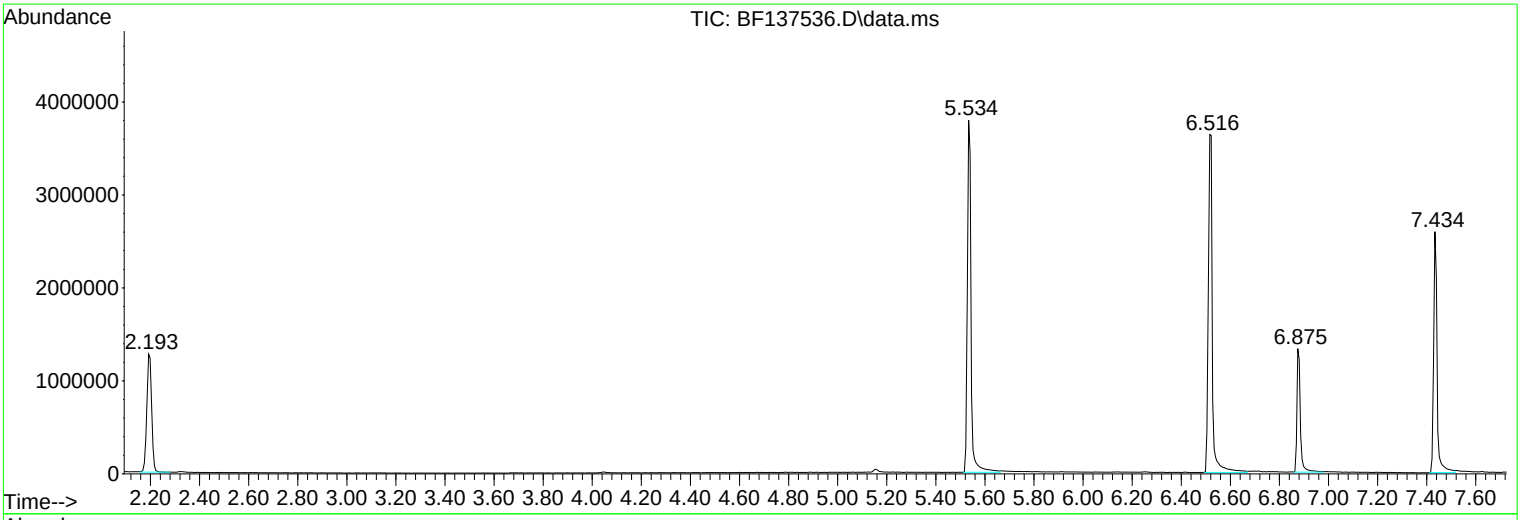
Sum of corrected areas: 36663670

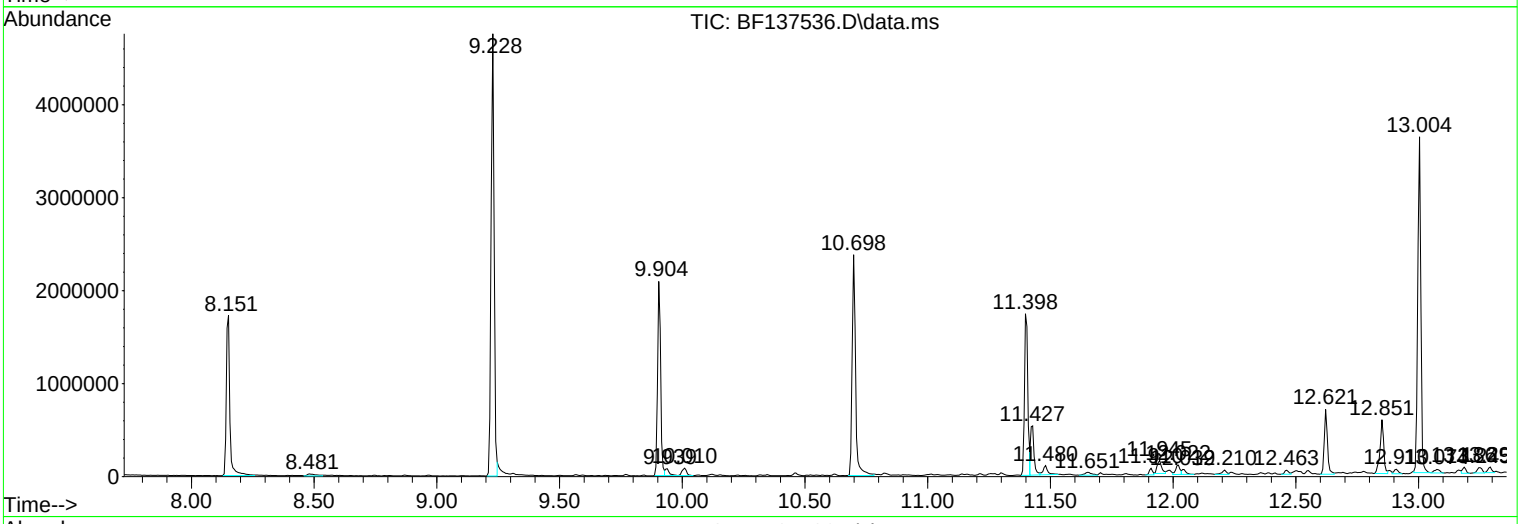
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030724\
Data File : BF137536.D
Acq On : 07 Mar 2024 18:19
Operator : CG\JU
Sample : P1688-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

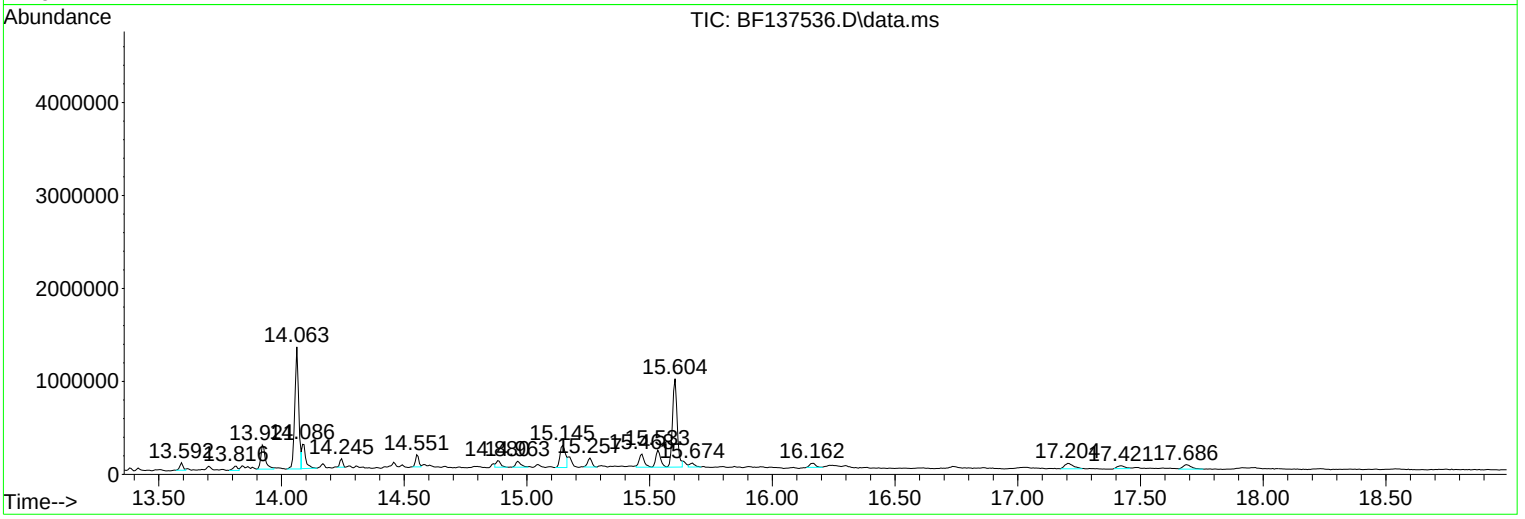
Instrument :
BNA_F
ClientSampleId :
COMP-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.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\BF030724\
Data File : BF137536.D
Acq On : 07 Mar 2024 18:19
Operator : CG\JU
Sample : P1688-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

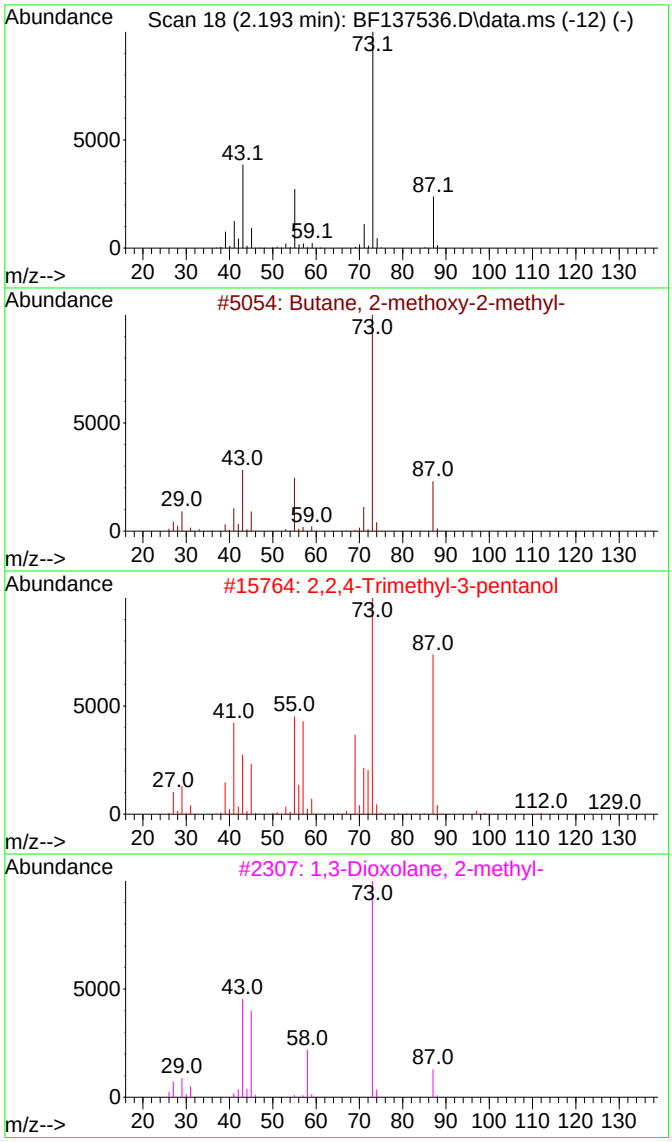
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

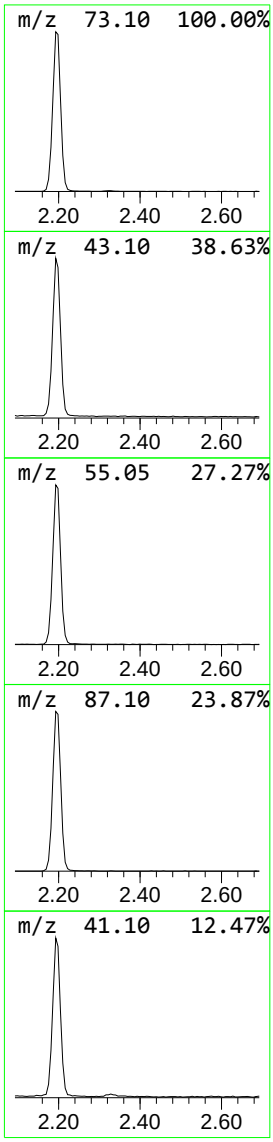
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.193	26.93 ng	1739190	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030724\
Data File : BF137536.D
Acq On : 07 Mar 2024 18:19
Operator : CG\JU
Sample : P1688-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

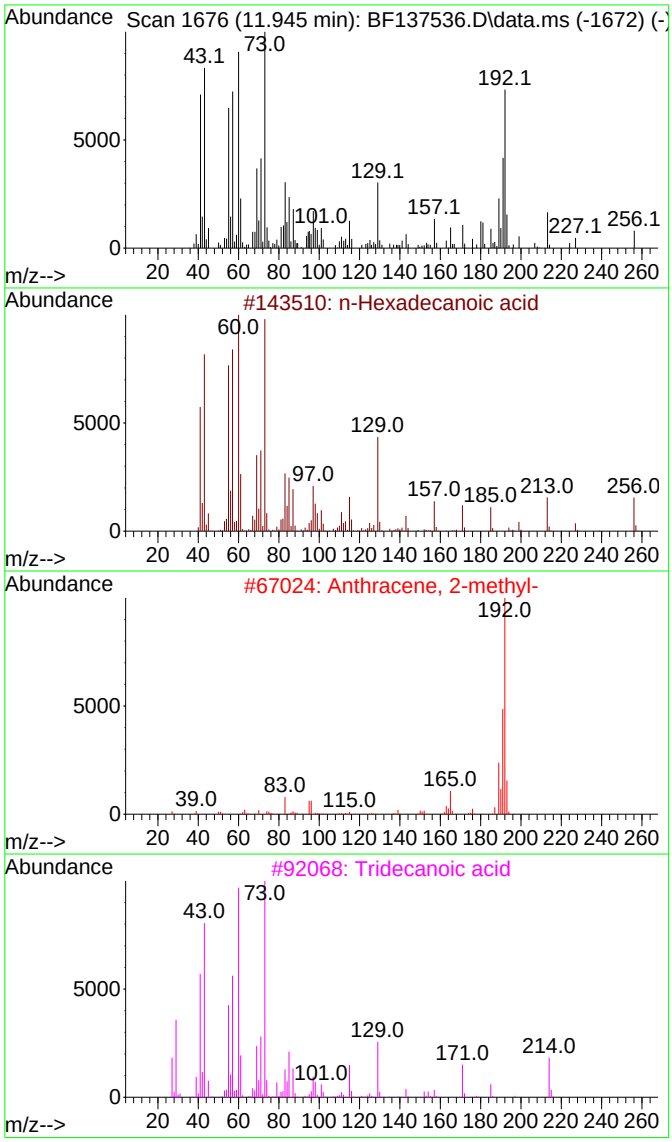
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

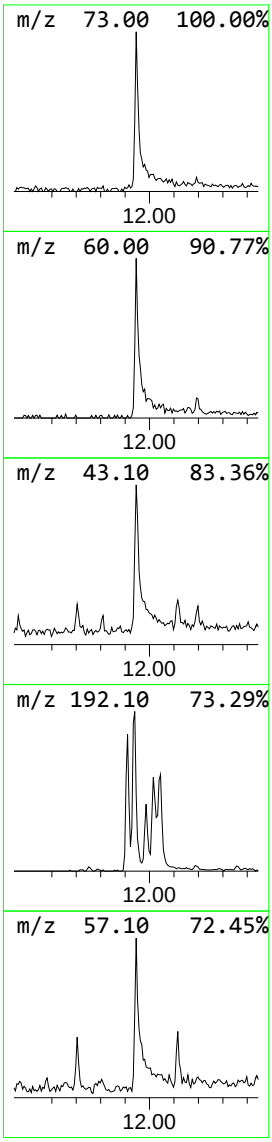
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	2.13 ng	178289	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	78
3	Tridecanoic acid	214	C13H26O2	000638-53-9	64
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	52
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	52





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030724\
Data File : BF137536.D
Acq On : 07 Mar 2024 18:19
Operator : CG\JU
Sample : P1688-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-5

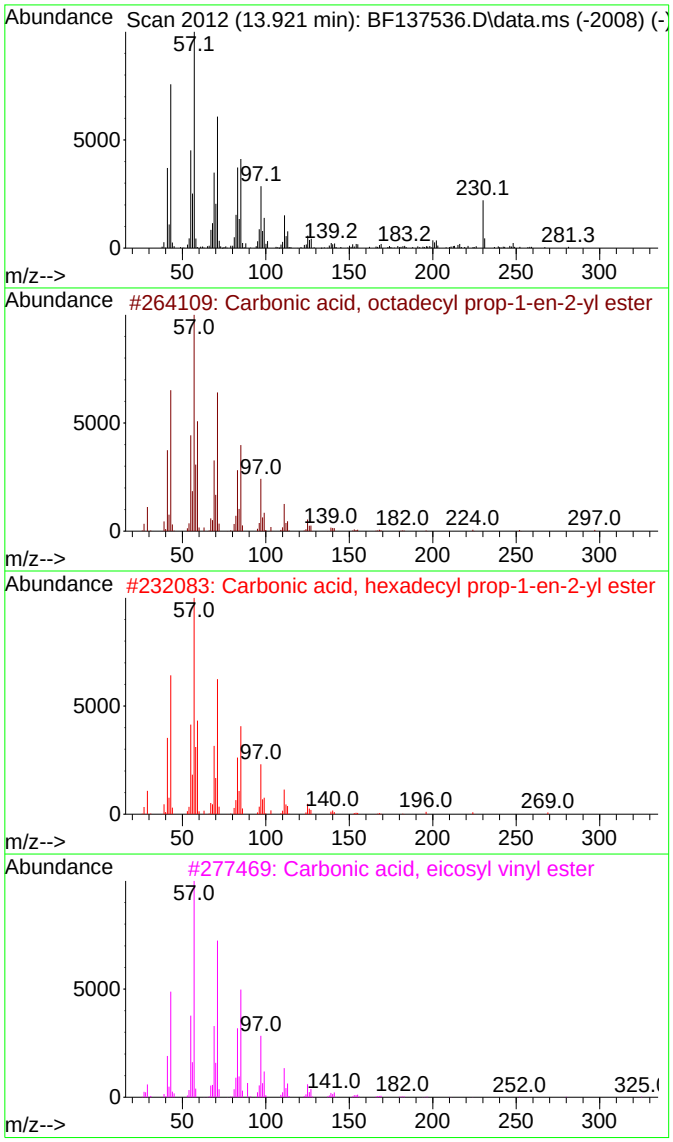
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

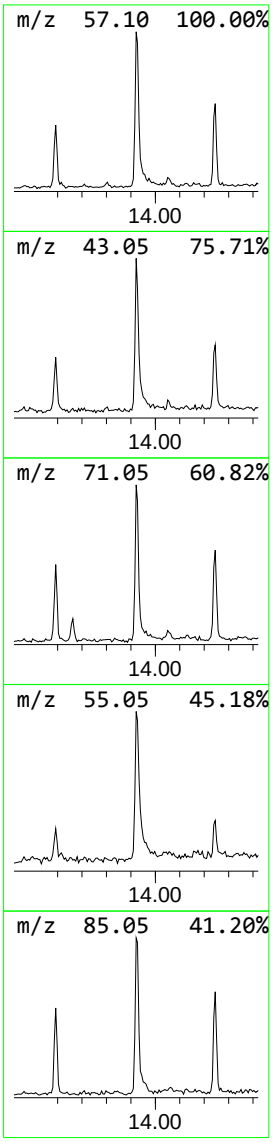
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Carbonic acid, octadecyl pr... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.921	4.69 ng	343000	Chrysene-d12	14.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	90
2	Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	90
3	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	87
4	Carbonic acid, octadecyl vinyl e...	340	C21H40O3	1000382-54-4	83
5	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030724\
Data File : BF137536.D
Acq On : 07 Mar 2024 18:19
Operator : CG\JU
Sample : P1688-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

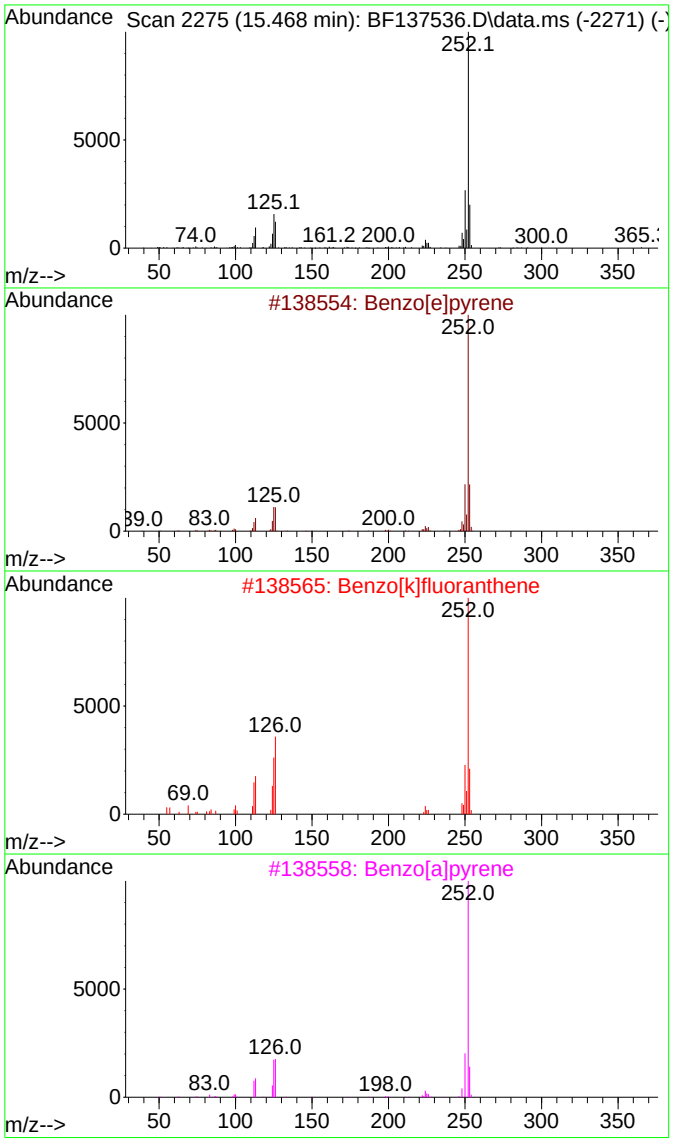
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

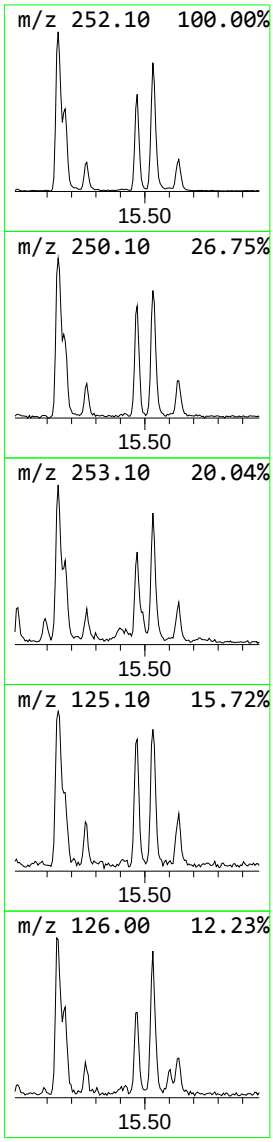
****

Peak Number 4 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.468	3.18 ng	202735	Perylene-d12	15.604

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	95
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
3	Benzo[a]pyrene	252	C20H12	000050-32-8	93
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	90
5	Perylene	252	C20H12	000198-55-0	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030724\
Data File : BF137536.D
Acq On : 07 Mar 2024 18:19
Operator : CG\JU
Sample : P1688-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

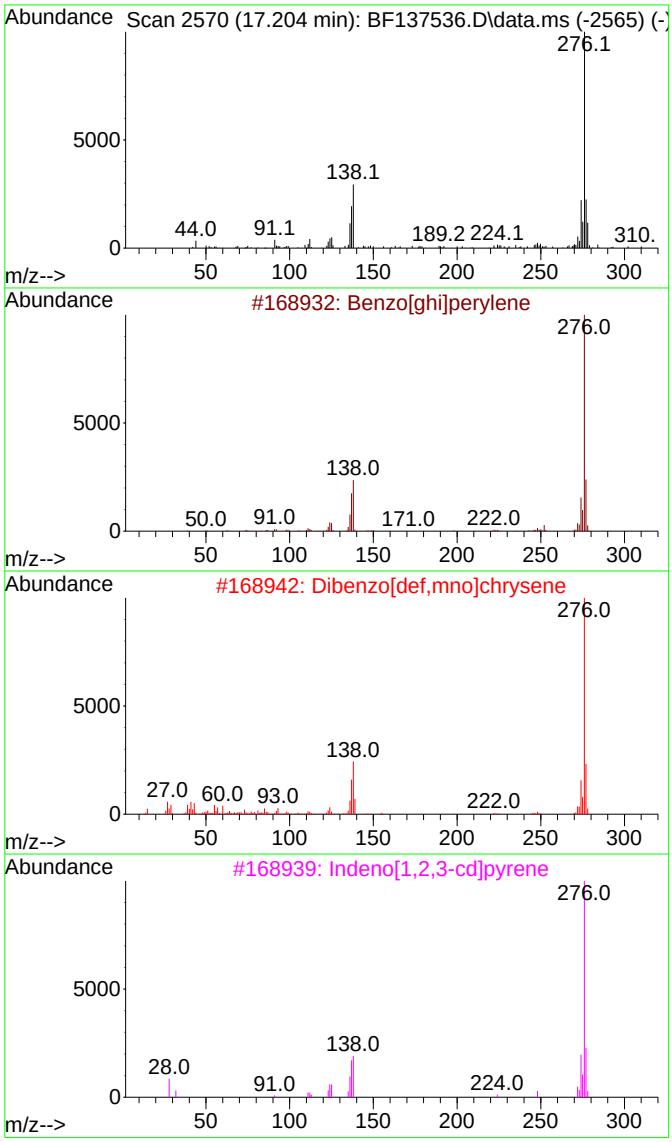
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

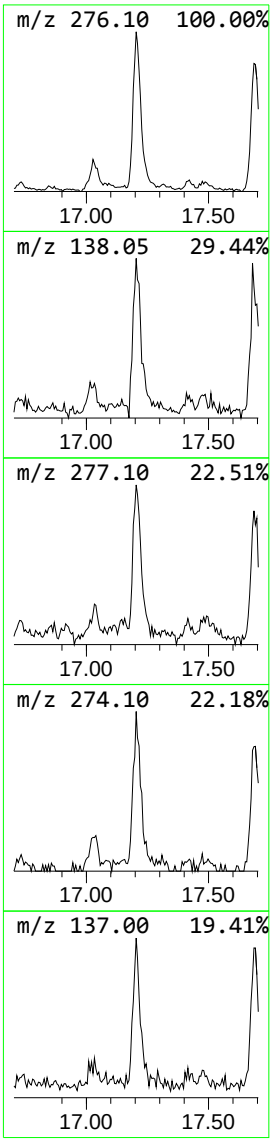
****

Peak Number 5 Dibenzo[def,mno]chrysene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.203	2.26 ng	144140	Perylene-d12	15.604

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[ghi]perylene	276	C22H12	000191-24-2	96
2	Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	93
3	Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	90
4	Indeno[1,2,3-cd]fluoranthene	276	C22H12	000193-43-1	90
5	2-Amino-3-cyano-4,5-diphenylthio...	276	C17H12N2S	042160-34-9	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030724\
Data File : BF137536.D
Acq On : 07 Mar 2024 18:19
Operator : CG\JU
Sample : P1688-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.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
Butane, 2-metho...	2.193	26.9	ng	1739190	1	6.875	1291660	20.0
n-Hexadecanoic ...	11.945	2.1	ng	178289	4	11.398	1671700	20.0
Carbonic acid, ...	13.921	4.7	ng	343000	5	14.063	1462130	20.0
Benzo[e]pyrene	15.468	3.2	ng	202735	6	15.604	1275940	20.0
Dibenzo[def,mno...	17.203	2.3	ng	144140	6	15.604	1275940	20.0