LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM071824\
Data File : BM046717.D
Acq On : 19 Jul 2024 00:40
Operator : MA/JU
Sample : P3246-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-CTW2-BL-03

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_M\Methods\8270-BM071724.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM046717.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.358	60	63	69	rBV	86842	106625	2.79%	0.343%
2	4.681	279	288	297	rBV	95260	140213	3.67%	0.450%
3	5.128	358	364	377	rBV	1740584	2388510	62.48%	7.673%
4	6.687	621	629	638	rBV	1727897	2577631	67.43%	8.281%
5	7.481	758	764	771	rVB	452731	689674	18.04%	2.216%
6	8.628	947	959	969	rBV	1120027	1751833	45.82%	5.628%
7	10.246	1226	1234	1240	rBV	536311	871025	22.78%	2.798%
8	10.998	1357	1362	1369	rBV	53801	92603	2.42%	0.297%
9	12.745	1652	1659	1667	rBV	2559696	3700499	96.80%	11.888%
10	14.128	1887	1894	1901	rBV	734294	1083348	28.34%	3.480%
11	14.192	1901	1905	1912	rVB	44699	65626	1.72%	0.211%
12	14.369	1929	1935	1936	rBV3	34518	51175	1.34%	0.164%
13	15.186	2067	2074	2079	rBV2	34897	55549	1.45%	0.178%
14	15.628	2142	2149	2158	rBV	2015819	2726345	71.32%	8.759%
15	16.880	2357	2362	2366	rBV	759163	1075306	28.13%	3.455%
16	16.928	2366	2370	2376	rVB	348666	486441	12.72%	1.563%
17	17.016	2381	2385	2392	rVB	93777	121709	3.18%	0.391%
18	17.292	2428	2432	2437	rVB	59832	82300	2.15%	0.264%
19	17.763	2507	2512	2515	rBV	47166	62959	1.65%	0.202%
20	17.816	2515	2521	2529	rVV3	347315	520648	13.62%	1.673%
21	17.951	2539	2544	2549	rBV3	62943	105498	2.76%	0.339%
22	18.269	2595	2598	2601	rBV	29535	40498	1.06%	0.130%
23	18.304	2601	2604	2609	rVB2	53217	67461	1.76%	0.217%
24	18.692	2666	2670	2676	rBV5	28080	43871	1.15%	0.141%
25	18.827	2689	2693	2699	rBV3	31513	52137	1.36%	0.167%
26	18.951	2709	2714	2720	rBV	657985	906898	23.72%	2.914%
27	19.110	2737	2741	2746	rBV3	141314	192767	5.04%	0.619%
28	19.316	2768	2776	2781	rBV	593248	917069	23.99%	2.946%
29	19.539	2809	2814	2825	rVB	3222798	3822926	100.00%	12.282%
30	19.821	2859	2862	2866	rVB	76843	83023	2.17%	0.267%
31	19.921	2876	2879	2884	rBV	54463	67193	1.76%	0.216%
32	20.851	3033	3037	3045	rVB3	284469	490137	12.82%	1.575%
33	21.110	3074	3081	3085	rBV3	995362	1767444	46.23%	5.678%
34	21.151	3085	3088	3097	rVB	344004	499412	13.06%	1.604%
35	21.892	3211	3214	3225	rVB6	188965	350152	9.16%	1.125%
36	23.009	3399	3404	3410	rBV	313663	760442	19.89%	2.443%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM071824\
Data File : BM046717.D
Acq On : 19 Jul 2024 00:40
Operator : MA/JU
Sample : P3246-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-CTW2-BL-03

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_M\Methods\8270-BM071724.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	23.621	3503	3508	3517	rVB	199439	458798	12.00%	1.474%
38	23.745	3523	3529	3536	rBV	268169	567230	14.84%	1.822%
39	23.874	3544	3551	3558	rBV	562767	1284224	33.59%	4.126%

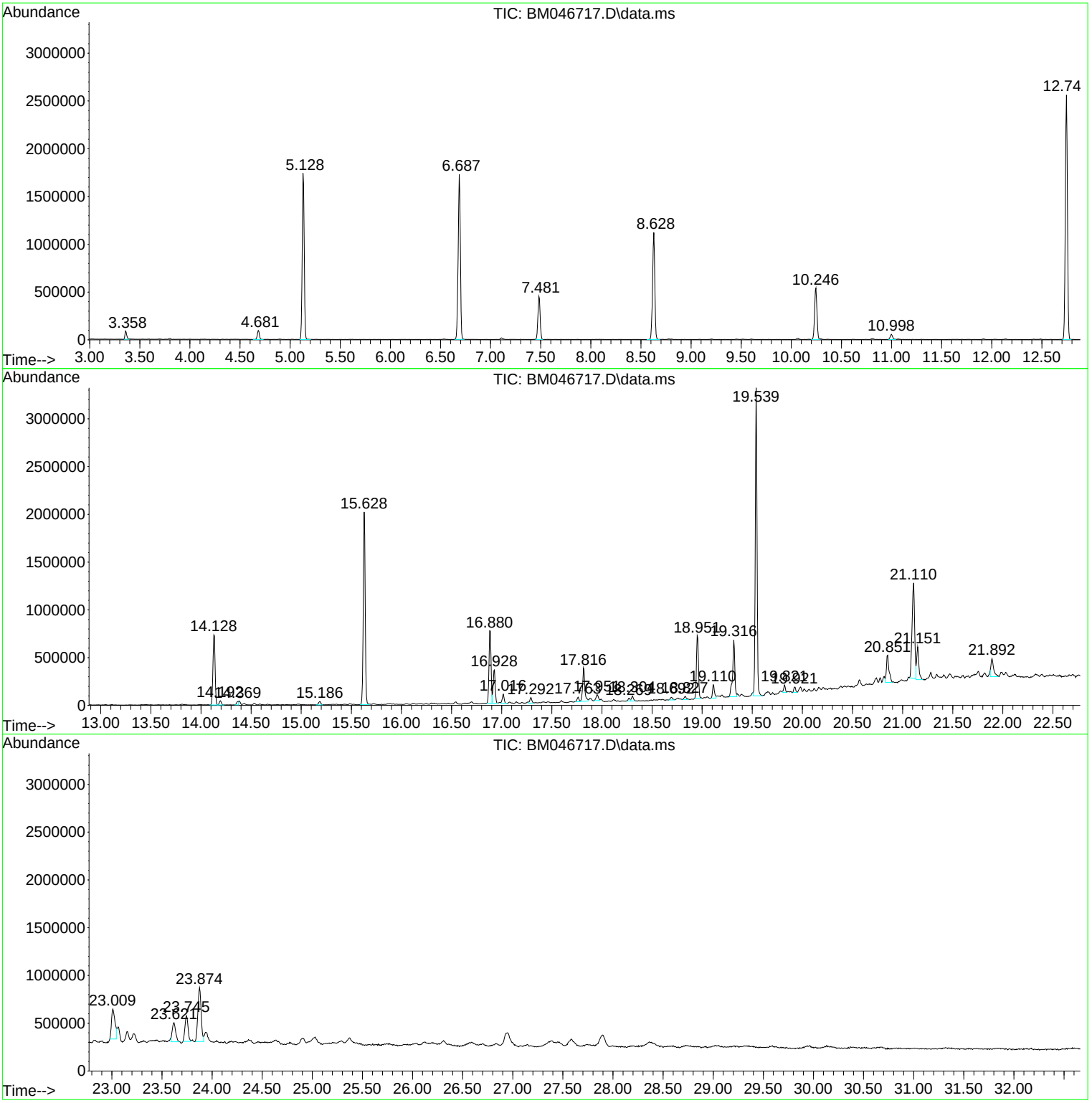
Sum of corrected areas: 31127199

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM071824\
Data File : BM046717.D
Acq On : 19 Jul 2024 00:40
Operator : MA/JU
Sample : P3246-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-CTW2-BL-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM071724.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_M\Data\BM071824\
Data File : BM046717.D
Acq On : 19 Jul 2024 00:40
Operator : MA/JU
Sample : P3246-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-CTW2-BL-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM071724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

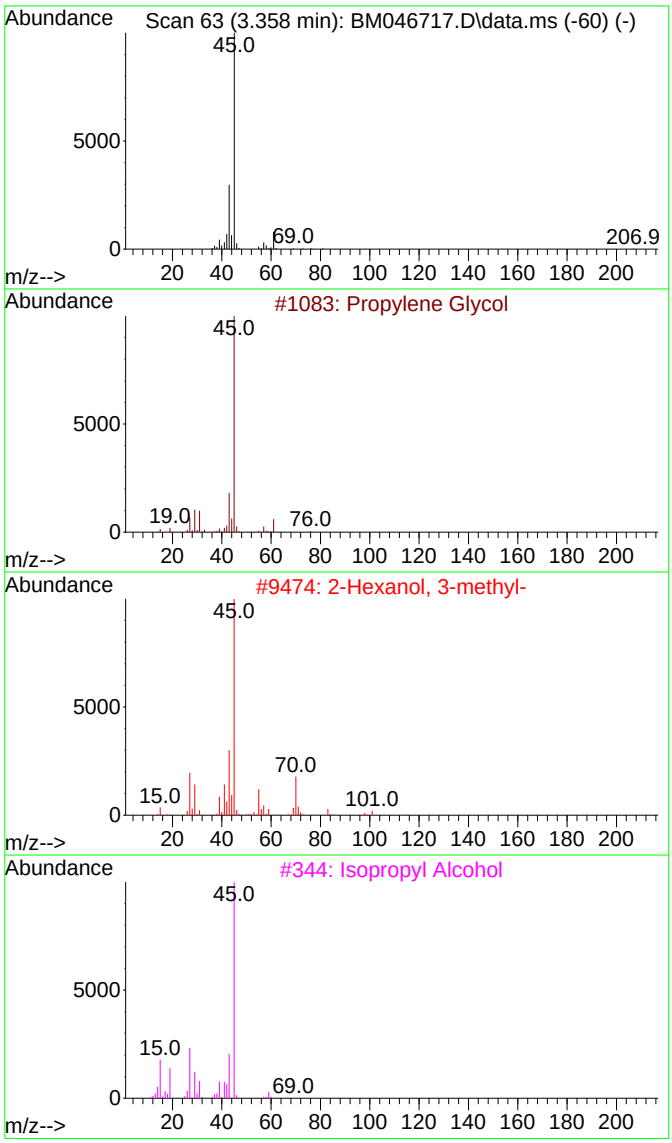
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

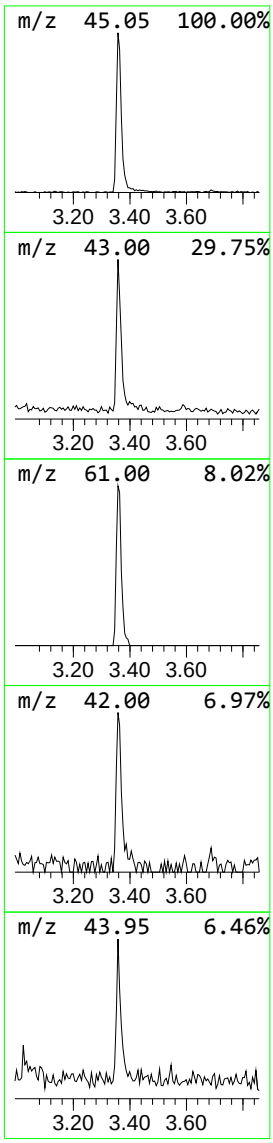
****

Peak Number 1 Propylene Glycol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.358	3.09 ng	106625	1,4-Dichlorobenzene-d4	7.481

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	78
2	2-Hexanol, 3-methyl-	116	C7H16O	002313-65-7	40
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4	Acetic acid, cyano-, 2-methoxyet...	143	C6H9NO3	010258-54-5	9
5	2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM071824\
Data File : BM046717.D
Acq On : 19 Jul 2024 00:40
Operator : MA/JU
Sample : P3246-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-CTW2-BL-03

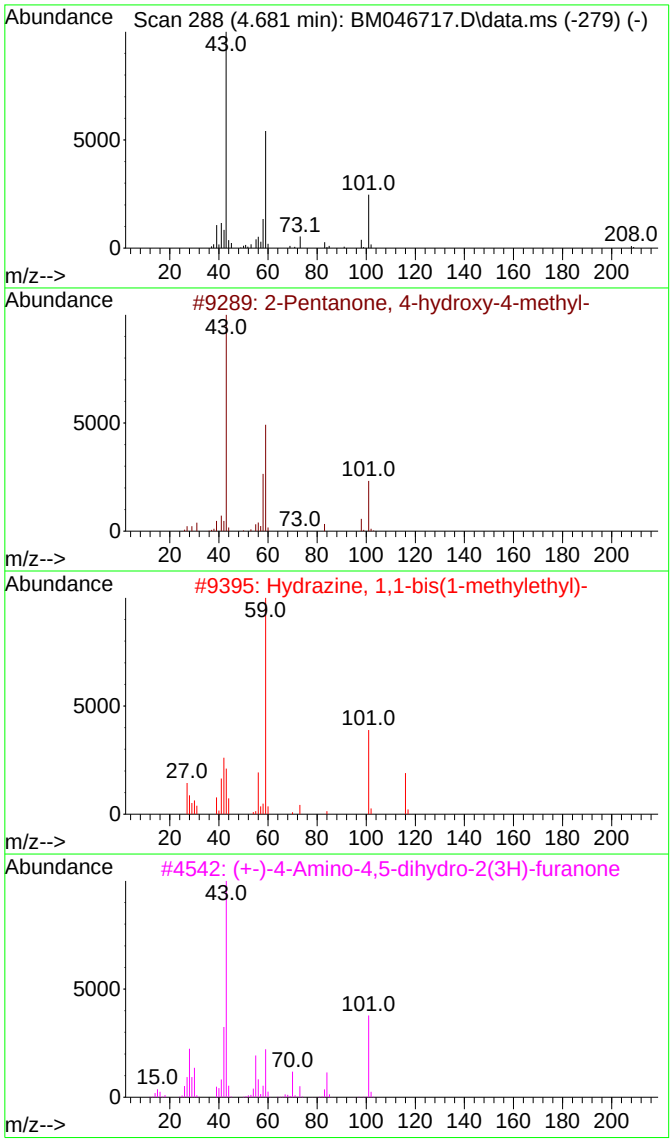
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM071724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

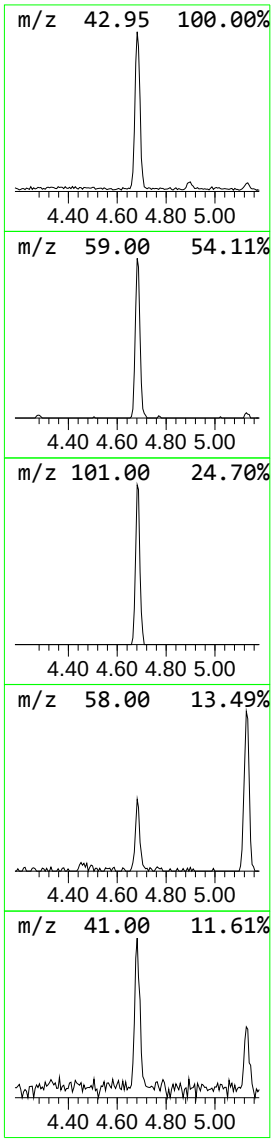
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.681	4.07 ng	140213	1,4-Dichlorobenzene-d4	7.481

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	40
3	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	38
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
5	Methyl 2,5,8,11-tetraoxatridecan...	236	C10H20O6	1000366-78-2	37





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM071824\
Data File : BM046717.D
Acq On : 19 Jul 2024 00:40
Operator : MA/JU
Sample : P3246-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-CTW2-BL-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM071724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

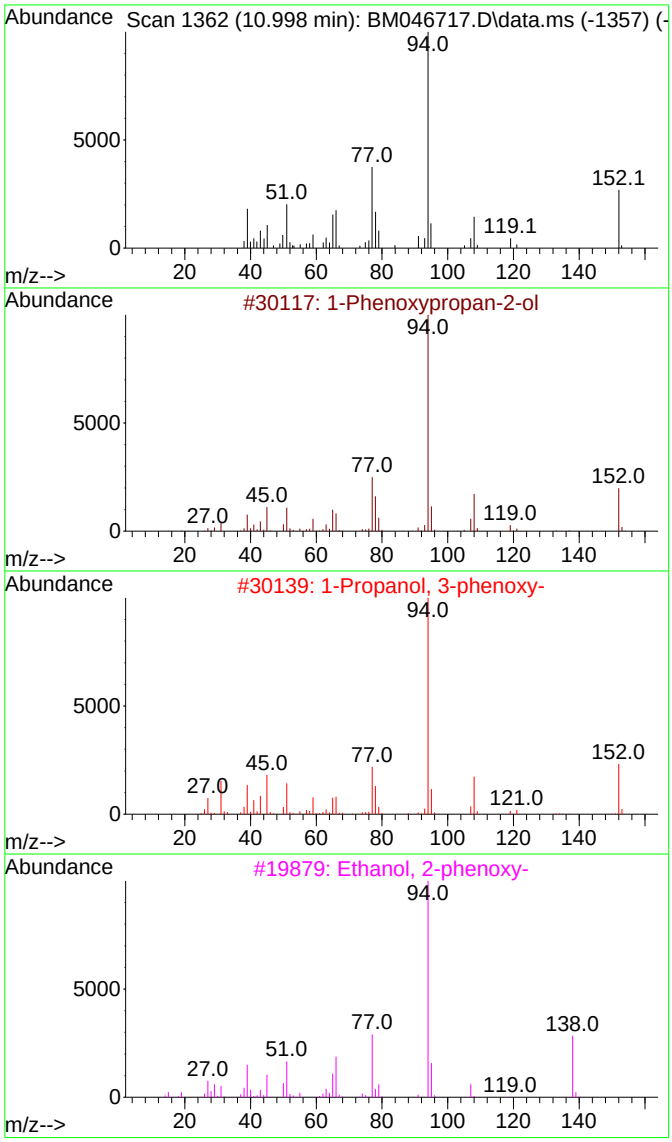
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

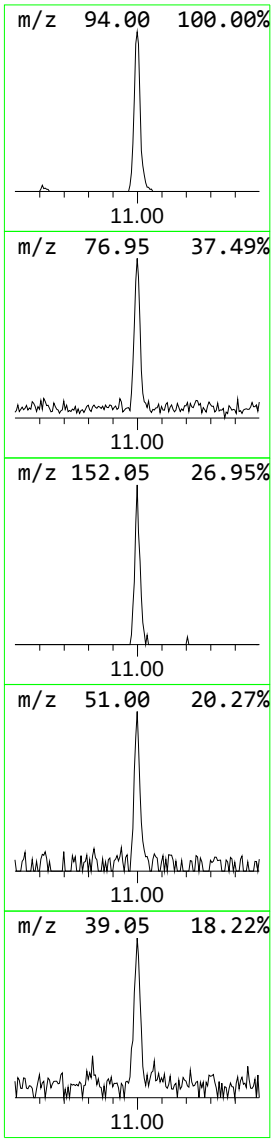
****

Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.999	2.13 ng	92603	Naphthalene-d8	10.246

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	91
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	80
3	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	53
4	2-Hexen-4-yne, 2-methyl-	94	C7H10	058275-93-7	50
5	Pyrimidine, 5-methyl-	94	C5H6N2	002036-41-1	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM071824\
Data File : BM046717.D
Acq On : 19 Jul 2024 00:40
Operator : MA/JU
Sample : P3246-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-CTW2-BL-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM071724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

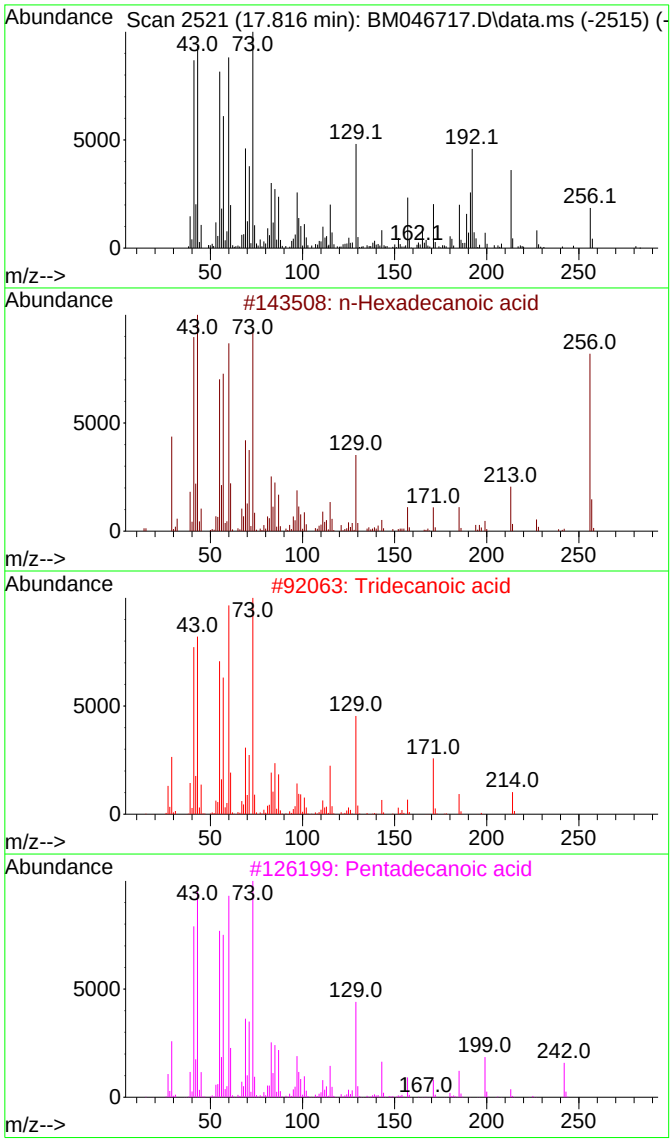
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

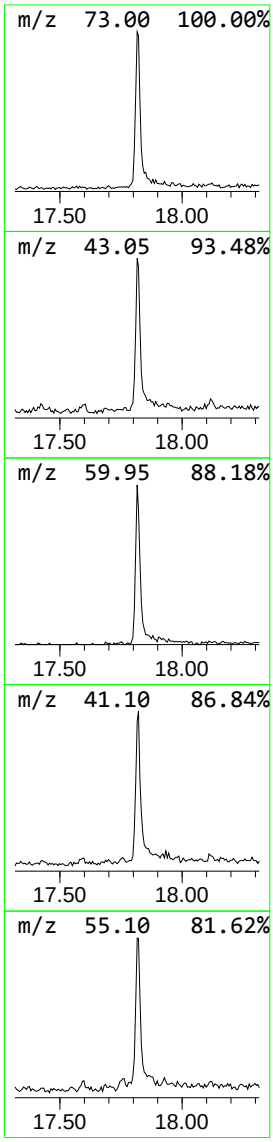
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.816	9.68 ng	520648	Phenanthrene-d10	16.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	49
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	46
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM071824\
Data File : BM046717.D
Acq On : 19 Jul 2024 00:40
Operator : MA/JU
Sample : P3246-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-CTW2-BL-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM071724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

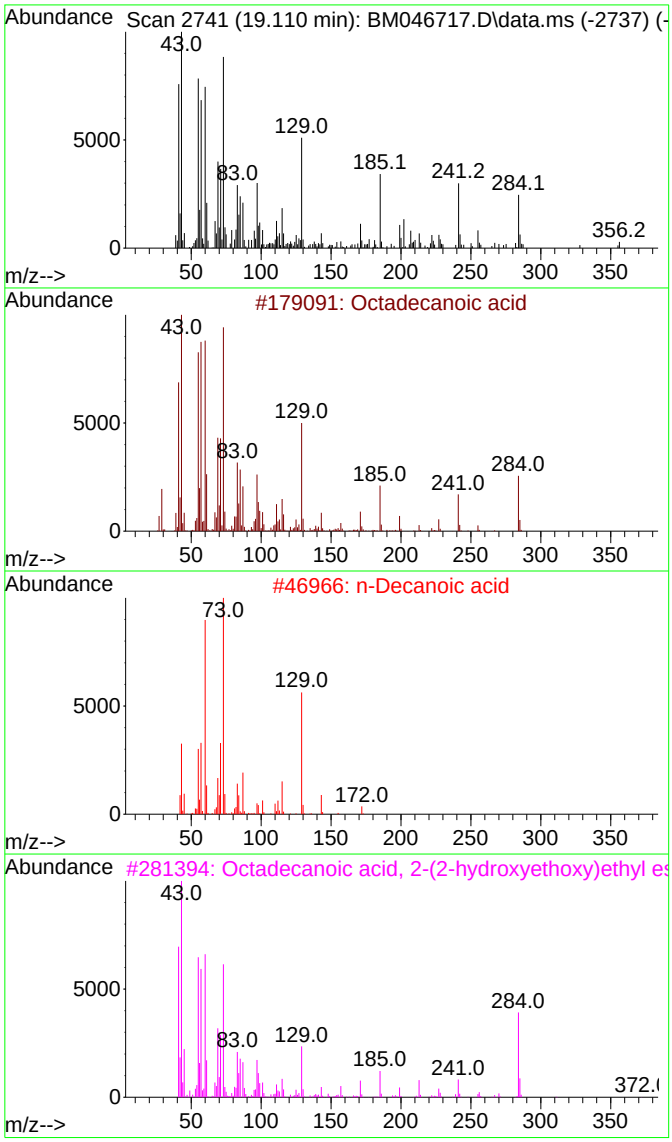
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

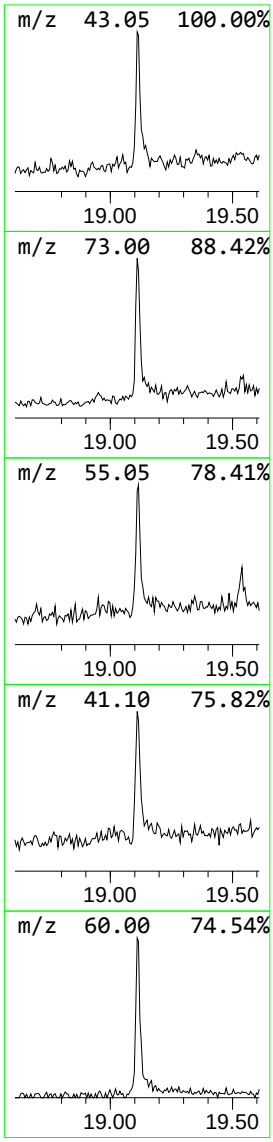
****

Peak Number 5 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.110	2.18 ng	192767	Chrysene-d12	21.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Decanoic acid	172	C10H20O2	000334-48-5	90
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM071824\
Data File : BM046717.D
Acq On : 19 Jul 2024 00:40
Operator : MA/JU
Sample : P3246-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-CTW2-BL-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM071724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

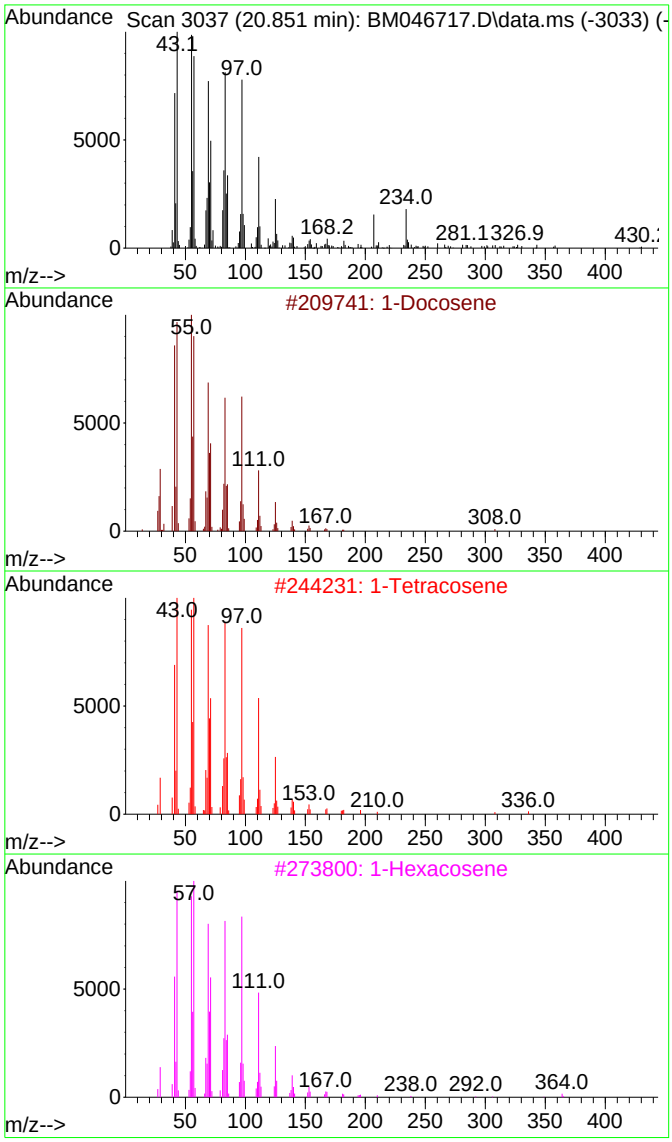
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

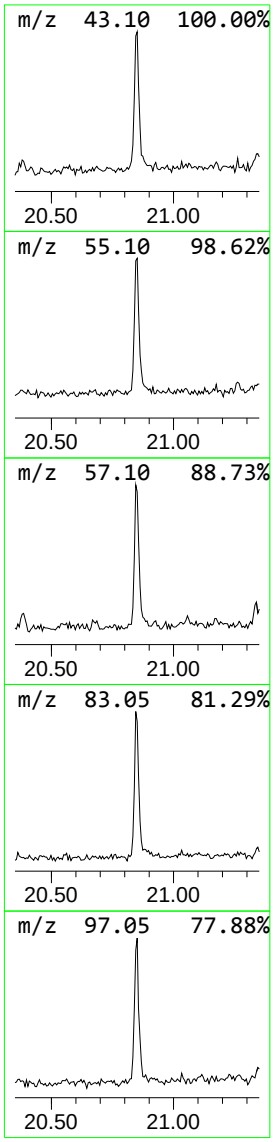
****

Peak Number 6 1-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.851	5.55 ng	490137	Chrysene-d12	21.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	99
2	1-Tetracosene	336	C24H48	010192-32-2	94
3	1-Hexacosene	364	C26H52	018835-33-1	94
4	1-Heptacosanol	396	C27H56O	002004-39-9	94
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM071824\
Data File : BM046717.D
Acq On : 19 Jul 2024 00:40
Operator : MA/JU
Sample : P3246-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-CTW2-BL-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM071724.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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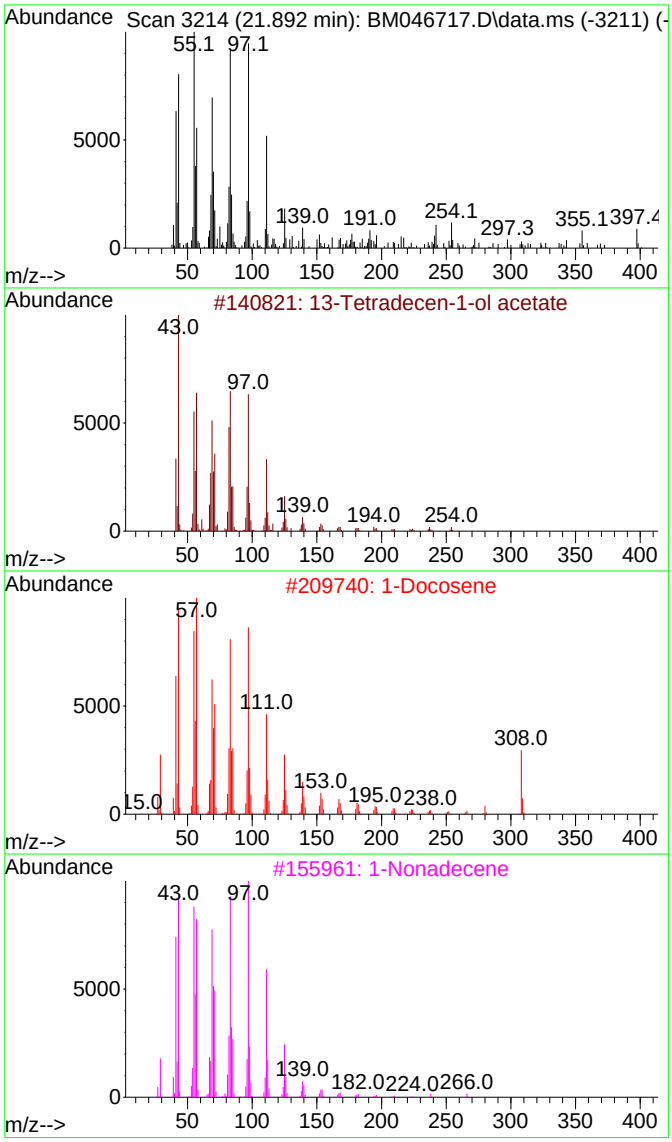
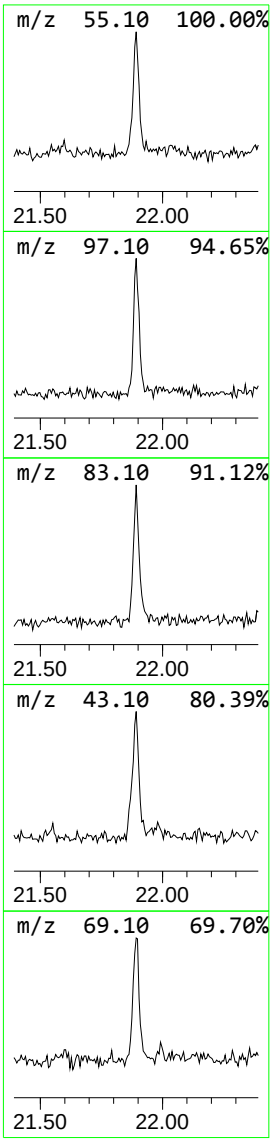
Peak Number 7 13-Tetradecen-1-ol acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.892	3.96 ng	350152	Chrysene-d12	21.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	86
2	1-Docosene	308	C22H44	001599-67-3	83
3	1-Nonadecene	266	C19H38	018435-45-5	83
4	1-Heneicosanol	312	C21H44O	015594-90-8	80
5	1-Tricosene	322	C23H46	018835-32-0	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM071824\
Data File : BM046717.D
Acq On : 19 Jul 2024 00:40
Operator : MA/JU
Sample : P3246-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-CTW2-BL-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM071724.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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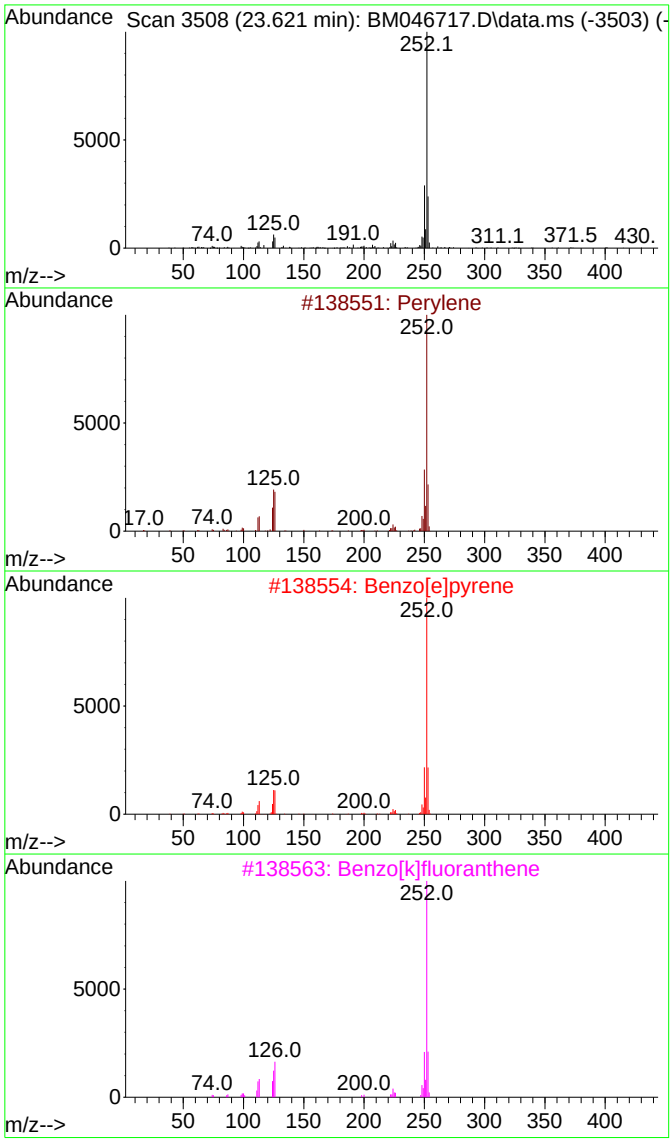
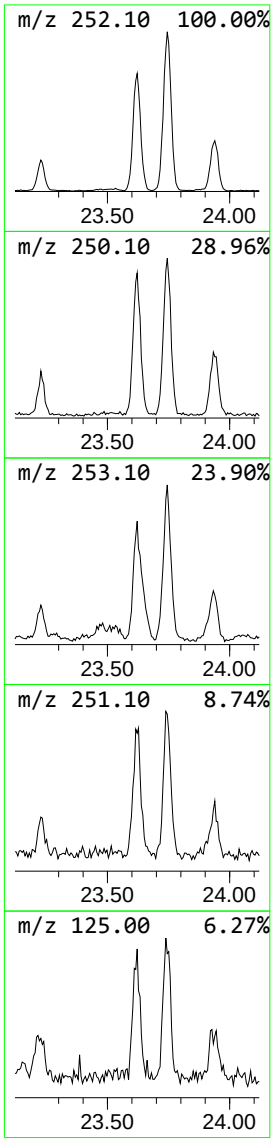
Peak Number 8 Perylene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.621	7.15 ng	458798	Perylene-d12	23.874

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





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM071824\
Data File : BM046717.D
Acq On : 19 Jul 2024 00:40
Operator : MA/JU
Sample : P3246-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-CTW2-BL-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM071724.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
Propylene Glycol	3.358	3.1	ng	106625	1	7.481	689674	20.0
2-Pentanone, 4-...	4.681	4.1	ng	140213	1	7.481	689674	20.0
1-Phenoxypropan...	10.999	2.1	ng	92603	2	10.246	871025	20.0
n-Hexadecanoic ...	17.816	9.7	ng	520648	4	16.881	1075310	20.0
Octadecanoic acid	19.110	2.2	ng	192767	5	21.110	1767440	20.0
1-Docosene	20.851	5.5	ng	490137	5	21.110	1767440	20.0
13-Tetradecen-1...	21.892	4.0	ng	350152	5	21.110	1767440	20.0
Perylene	23.621	7.2	ng	458798	6	23.874	1284220	20.0