LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM071824\
Data File : BM046716.D
Acq On : 19 Jul 2024 00:01
Operator : MA/JU
Sample : P3246-21
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-CTW2-BL-05

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: BM046716.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	75	rBV	87484	112286	2.38%	0.407%
2	4.687	282	289	295	rBV	114141	169229	3.59%	0.613%
3	5.134	357	365	371	rBV	2068671	2854459	60.51%	10.336%
4	6.687	621	629	639	rBV	2023427	3138736	66.54%	11.366%
5	7.481	758	764	773	rVB	393364	608030	12.89%	2.202%
6	8.628	951	959	968	rBV	1297110	2061102	43.70%	7.463%
7	10.245	1227	1234	1244	rVB	480139	764619	16.21%	2.769%
8	10.998	1357	1362	1370	rBV2	40743	70452	1.49%	0.255%
9	12.745	1652	1659	1666	rBV	3251053	4515868	95.74%	16.352%
10	14.128	1887	1894	1902	rVB	637244	964480	20.45%	3.492%
11	14.386	1929	1938	1944	rBV4	46040	109402	2.32%	0.396%
12	15.627	2143	2149	2161	rBV	2565740	3582768	75.96%	12.973%
13	16.886	2357	2363	2368	rBV	737306	1004076	21.29%	3.636%
14	17.821	2516	2522	2530	rBV	204656	312507	6.63%	1.132%
15	19.110	2737	2741	2747	rBV	82611	118406	2.51%	0.429%
16	19.539	2808	2814	2820	rBV	3940892	4716946	100.00%	17.080%
17	20.539	2980	2984	2989	rVB	410250	440938	9.35%	1.597%
18	20.851	3033	3037	3044	rVB	147846	196806	4.17%	0.713%
19	21.109	3076	3081	3086	rBV	661210	888873	18.84%	3.219%
20	23.874	3544	3551	3560	rVB	437221	986361	20.91%	3.572%

Sum of corrected areas: 27616344

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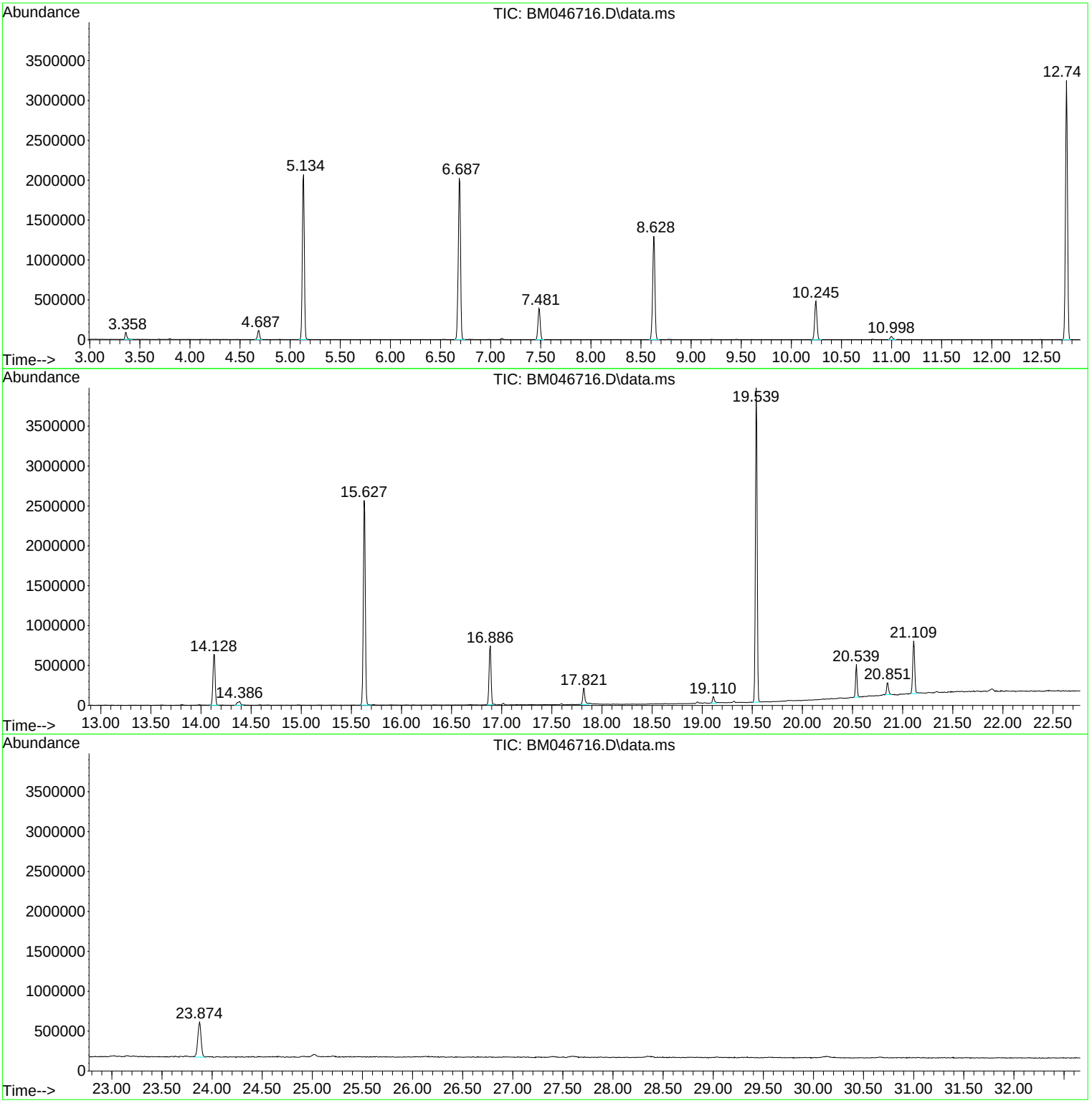
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-CTW2-BL-05

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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Data File : BM046716.D
Acq On : 19 Jul 2024 00:01
Operator : MA/JU
Sample : P3246-21
Misc :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

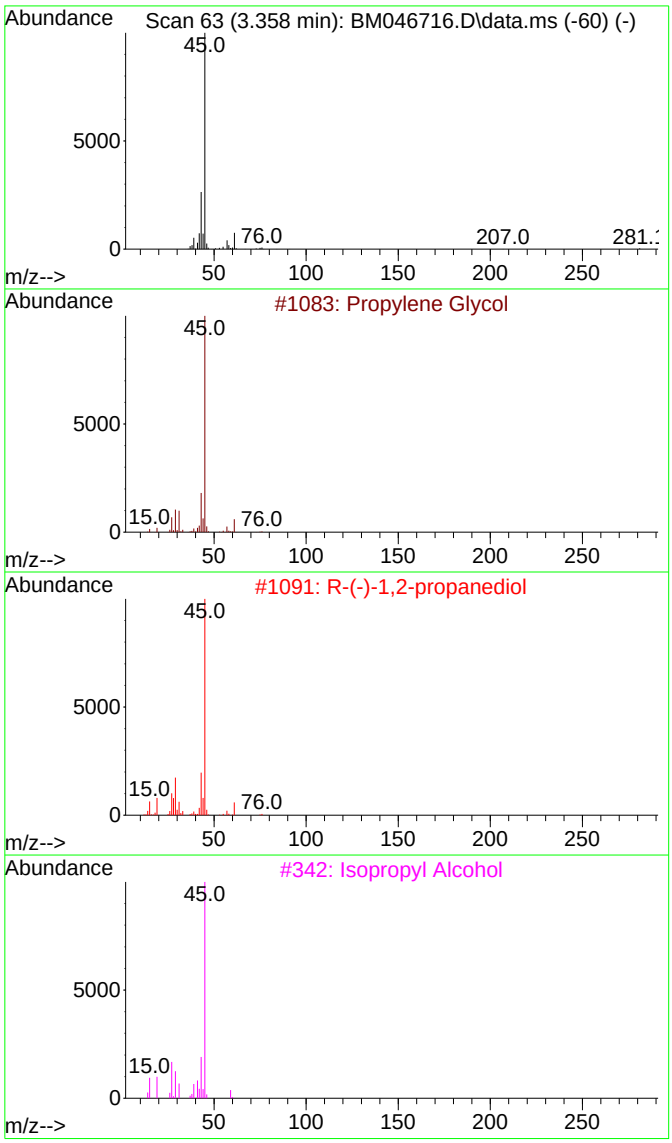
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

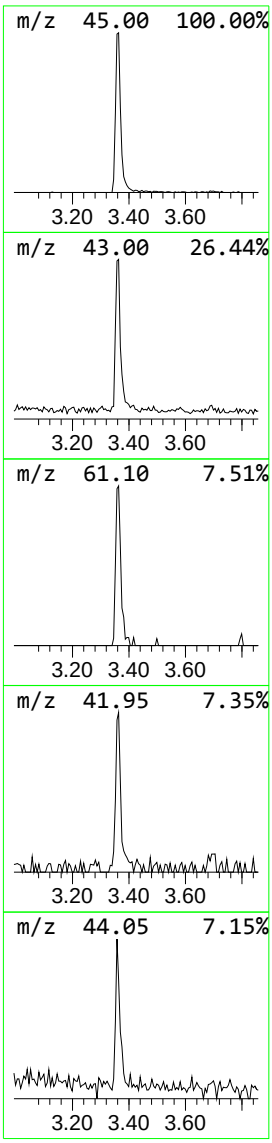
****

Peak Number 1 Propylene Glycol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.358	3.69 ng	112286	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	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	50
4	2-Hexanol, 3-methyl-	116	C7H16O	002313-65-7	40
5	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	40





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Data File : BM046716.D
Acq On : 19 Jul 2024 00:01
Operator : MA/JU
Sample : P3246-21
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-CTW2-BL-05

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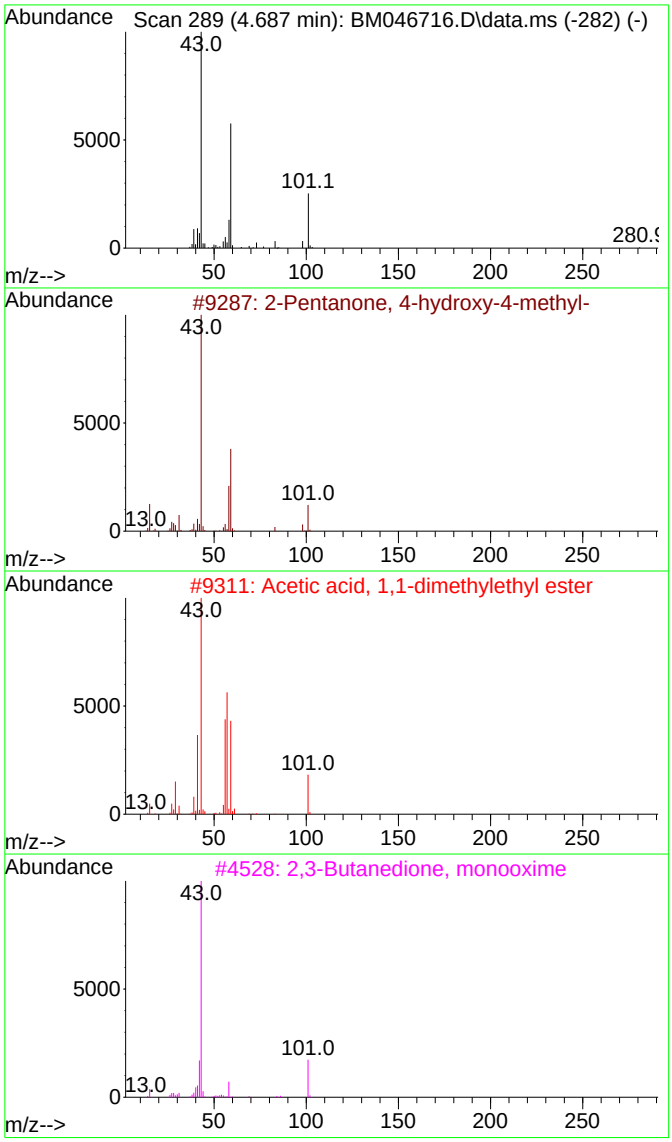
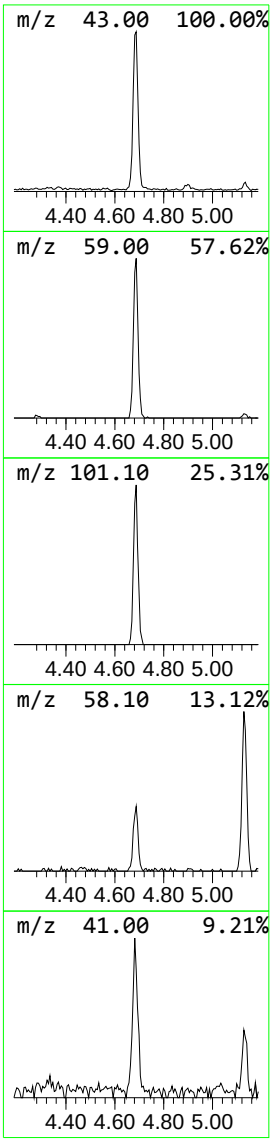
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.687	5.57 ng	169229	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	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	Silane, trimethyl-	74	C3H10Si	000993-07-7	17
5	5-Hexen-2-one	98	C6H10O	000109-49-9	10





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Acq On : 19 Jul 2024 00:01
Operator : MA/JU
Sample : P3246-21
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-CTW2-BL-05

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
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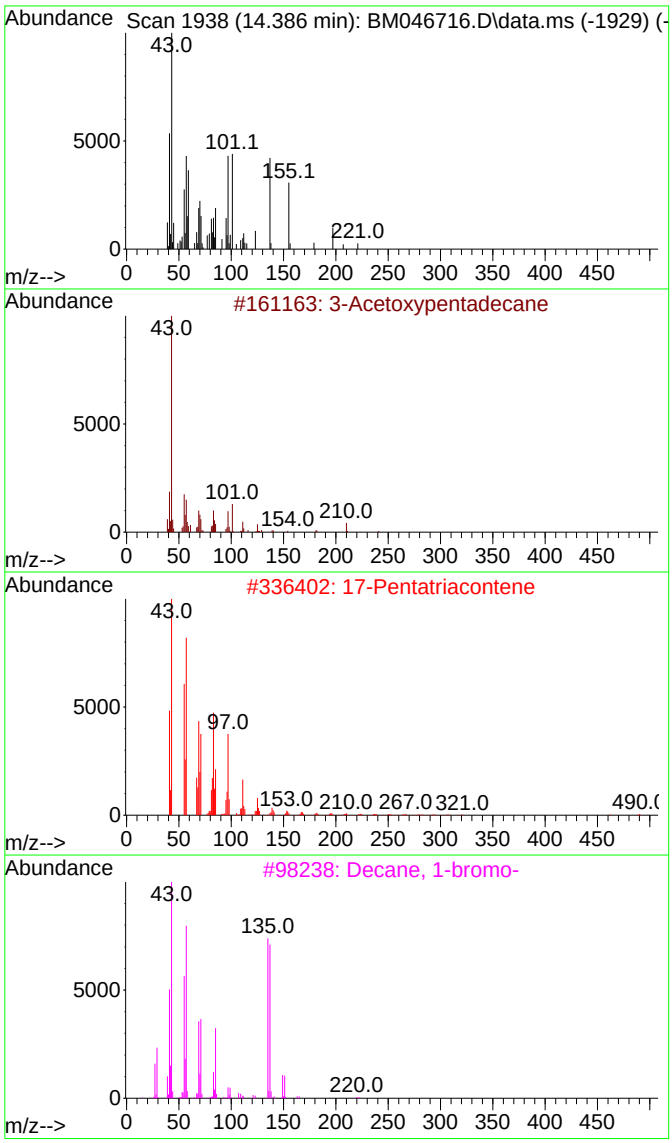
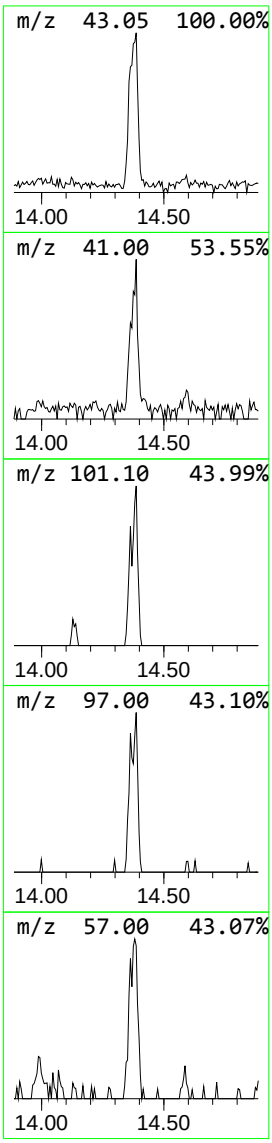
Peak Number 3 unknown14.386 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.386	2.27 ng	109402	Acenaphthene-d10	14.128

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Acetoxypentadecane	270	C17H34O2	1000245-62-1	43
2	17-Pentatriacontene	491	C35H70	006971-40-0	12
3	Decane, 1-bromo-	220	C10H21Br	000112-29-8	9
4	1-Nonadecene	266	C19H38	018435-45-5	9
5	1H-Pyrrole-2,5-dione	97	C4H3NO2	000541-59-3	9





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Operator : MA/JU
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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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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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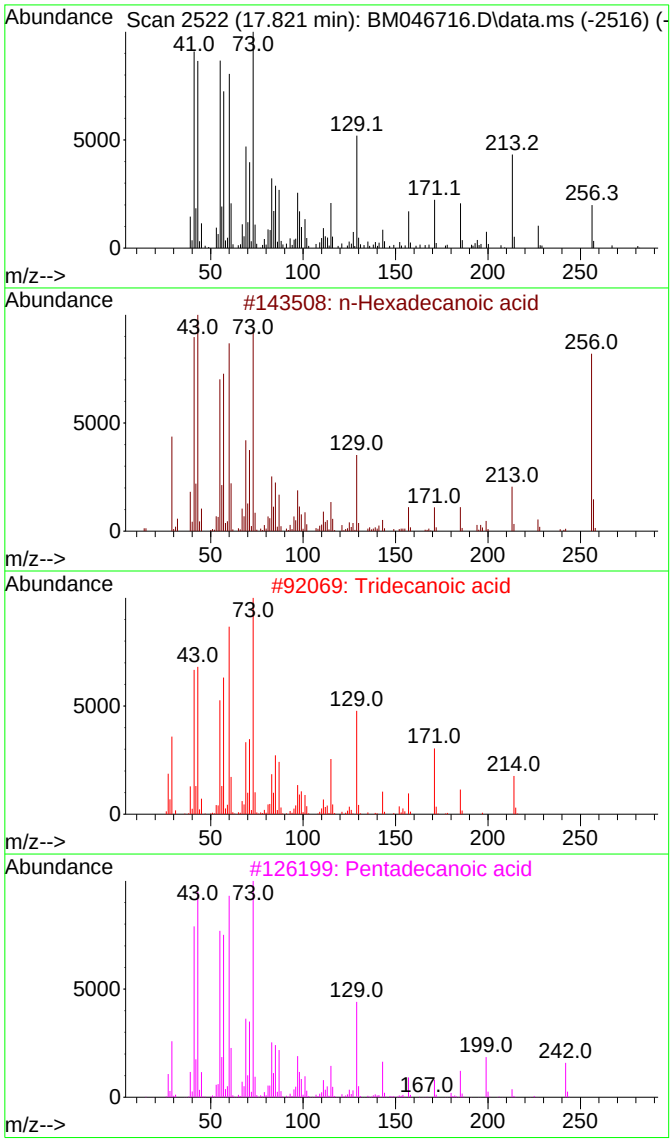
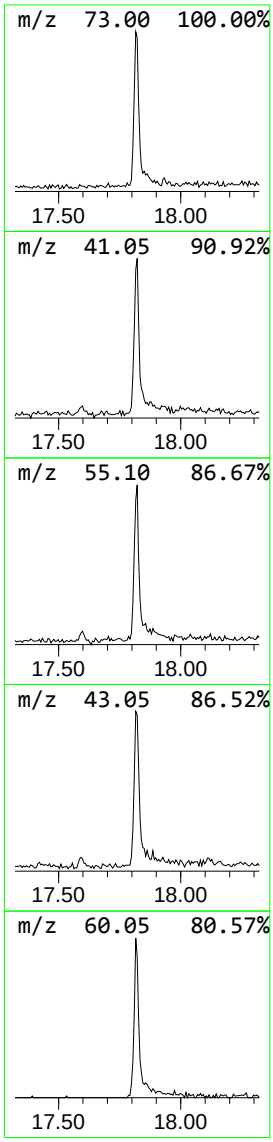
Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.822	6.22 ng	312507	Phenanthrene-d10	16.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	86
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	58
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	47
5	Undecanoic acid	186	C11H22O2	000112-37-8	43





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Operator : MA/JU
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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-CTW2-BL-05

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
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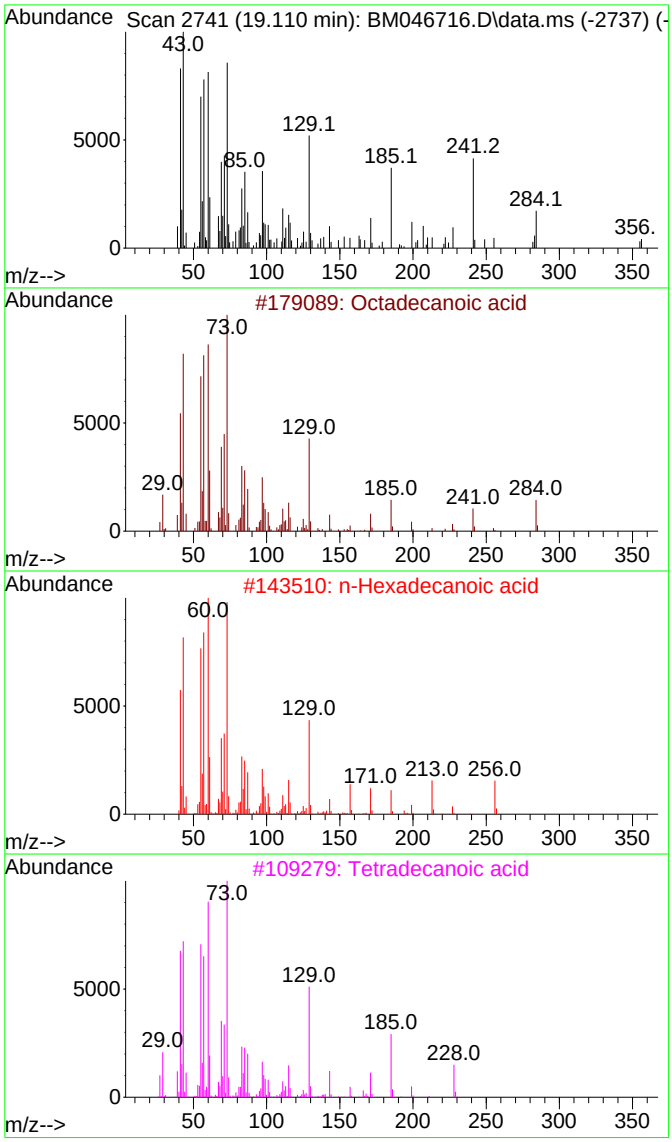
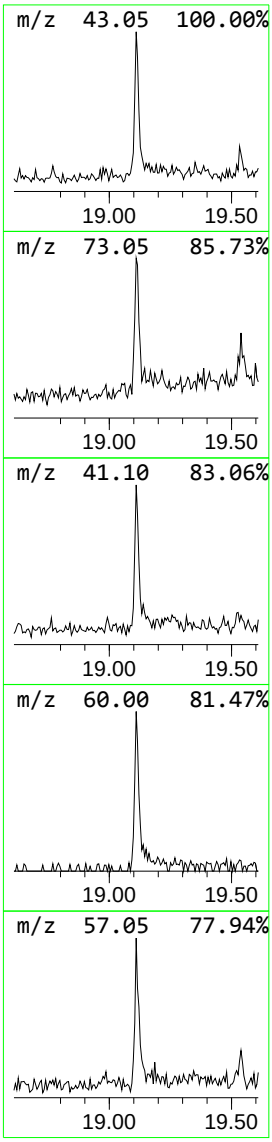
Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.110	2.66 ng	118406	Chrysene-d12	21.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	62
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	50
5	Tridecanoic acid	214	C13H26O2	000638-53-9	46





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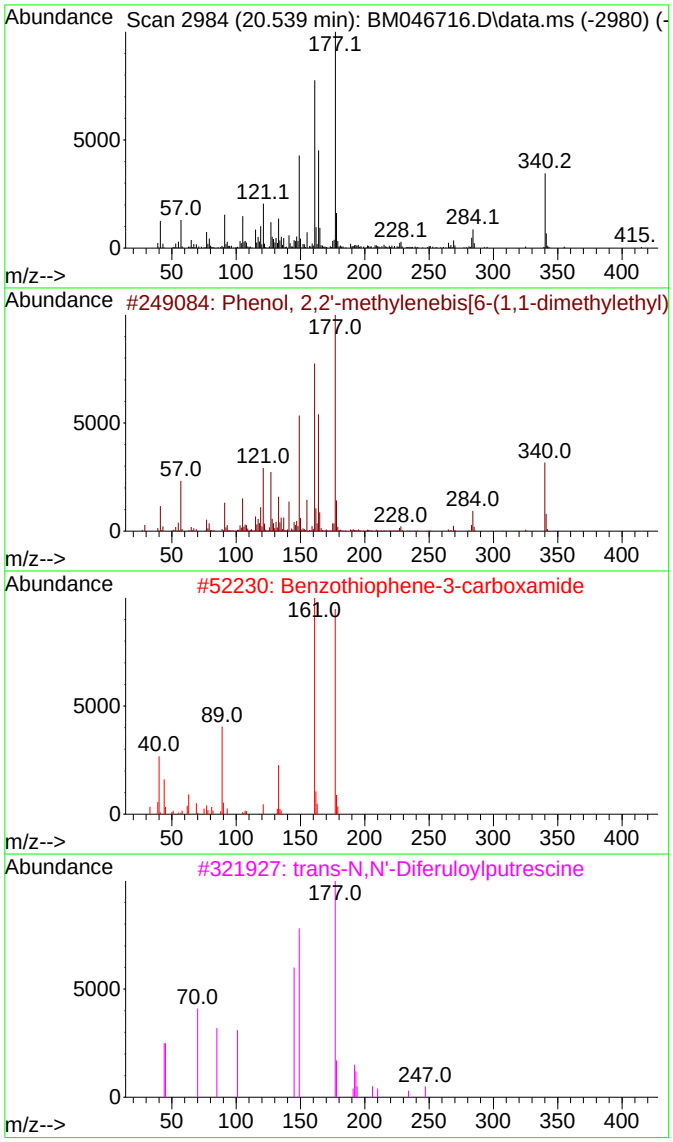
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM071724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

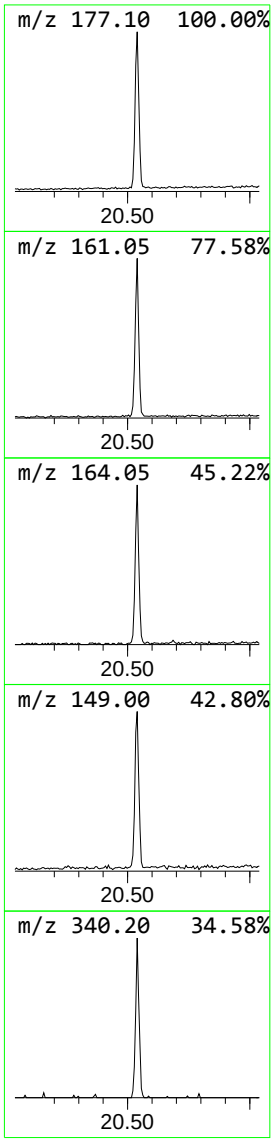
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Phenol, 2,2'-methylenebis[6... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.539	9.92 ng	440938	Chrysene-d12	21.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,2'-methylenebis[6-(1,1...	340	C23H32O2	000119-47-1	91
2	Benzothiophene-3-carboxamide	177	C9H7NOS	1000262-24-0	47
3	trans-N,N'-Diferuloylputrescine	440	C24H28N2O6	042369-86-8	30
4	benzenemethanesulfonamide, N-[4-...	332	C18H24N2O2S	1000402-41-3	25
5	Benzenamine, 2,6-dichloro-	161	C6H5Cl2N	000608-31-1	22





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TIC Library : C:\Database\NIST20.L
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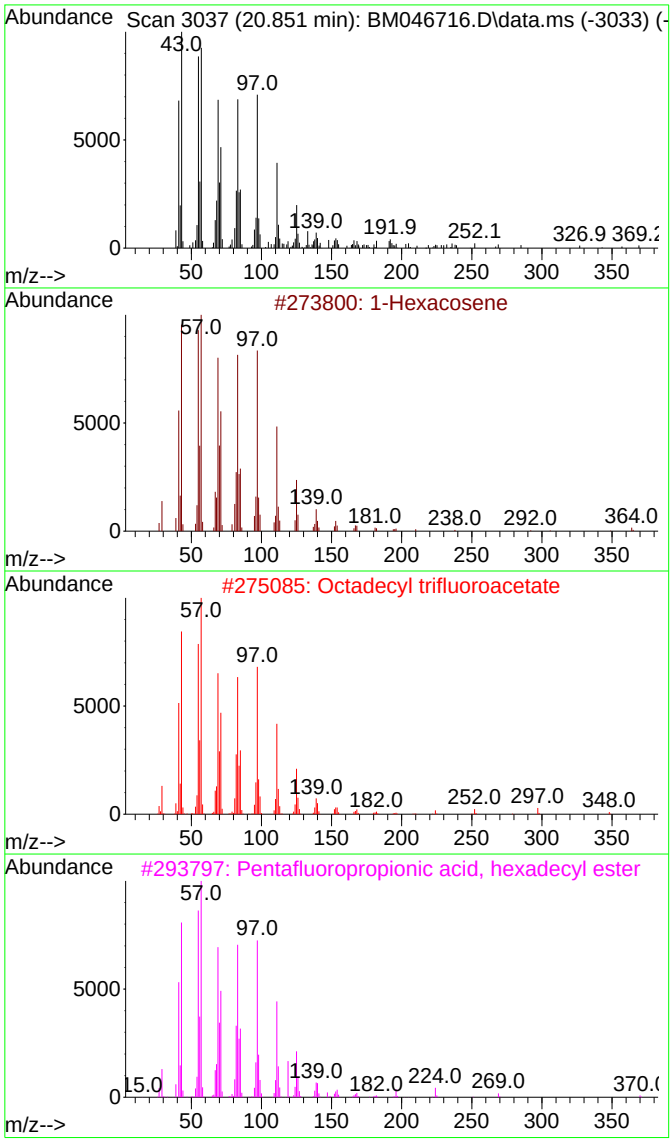
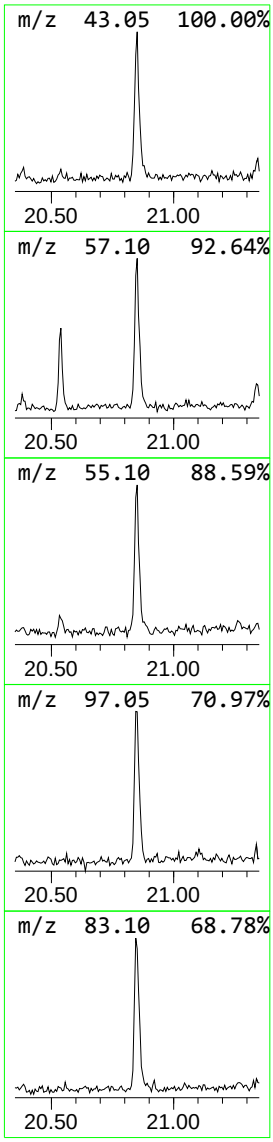
Peak Number 7 1-Hexacosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.851	4.43 ng	196806	Chrysene-d12	21.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene	364	C26H52	018835-33-1	95
2	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	95
3	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	94
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	94





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propylene Glycol	3.358	3.7	ng	112286	1	7.481	608030	20.0
2-Pentanone, 4-...	4.687	5.6	ng	169229	1	7.481	608030	20.0
unknown14.386	14.386	2.3	ng	109402	3	14.128	964480	20.0
n-Hexadecanoic ...	17.822	6.2	ng	312507	4	16.886	1004080	20.0
Octadecanoic acid	19.110	2.7	ng	118406	5	21.110	888873	20.0
Phenol, 2,2'-me...	20.539	9.9	ng	440938	5	21.110	888873	20.0
1-Hexacosene	20.851	4.4	ng	196806	5	21.110	888873	20.0