LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080723\
Data File : BM041311.D
Acq On : 07 Aug 2023 14:20
Operator : MA/JU
Sample : 03903-18
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-08W

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-BM072823.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM041311.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.363	363	370	387	rBV	1417352	2071940	18.41%	4.558%
2	6.969	637	643	659	rBV	821367	1324463	11.77%	2.914%
3	7.787	775	782	790	rBV	502572	790820	7.03%	1.740%
4	8.969	975	983	999	rBV	1866528	3056523	27.16%	6.724%
5	10.592	1250	1259	1274	rBV	681359	1170695	10.40%	2.575%
6	13.075	1673	1681	1693	rBV	5293218	7336850	65.18%	16.139%
7	14.457	1909	1916	1926	rBV	1110264	1664591	14.79%	3.662%
8	15.292	2053	2058	2063	rVB	114988	143320	1.27%	0.315%
9	15.827	2145	2149	2160	rVB	144054	210279	1.87%	0.463%
10	15.957	2161	2171	2189	rBV	4514367	6380547	56.69%	14.036%
11	16.163	2201	2206	2223	rVB	204495	387708	3.44%	0.853%
12	16.957	2337	2341	2345	rBV	220666	254166	2.26%	0.559%
13	17.216	2379	2385	2390	rBV	1570751	2147929	19.08%	4.725%
14	17.698	2463	2467	2473	rBV	202373	245548	2.18%	0.540%
15	18.115	2532	2538	2548	rBV	972940	1444124	12.83%	3.177%
16	18.398	2582	2586	2592	rBV	157965	188539	1.68%	0.415%
17	19.033	2691	2694	2698	rVB	111008	123157	1.09%	0.271%
18	19.398	2752	2756	2764	rBV	536352	744448	6.61%	1.638%
19	19.857	2828	2834	2839	rBV	9650842	11255429	100.00%	24.759%
20	21.127	3046	3050	3060	rVB2	317628	457042	4.06%	1.005%
21	21.421	3095	3100	3110	rBV	1735356	2175561	19.33%	4.786%
22	23.792	3497	3503	3510	rVB	1002123	1885809	16.75%	4.148%

Sum of corrected areas: 45459488

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080723\
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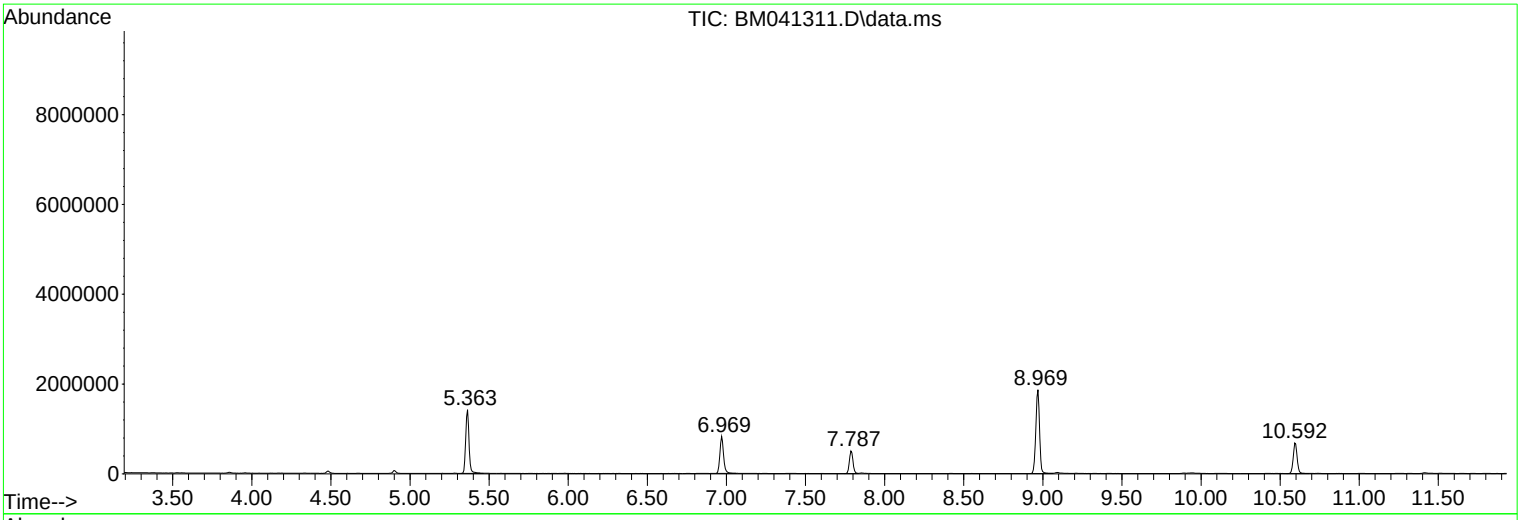
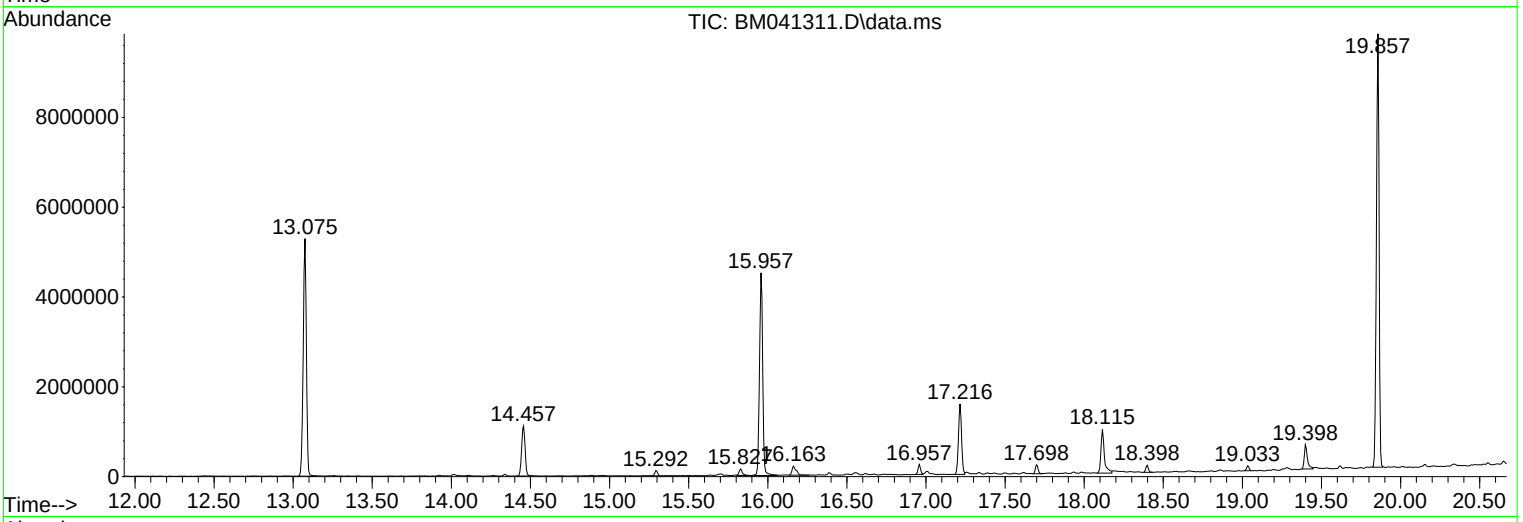
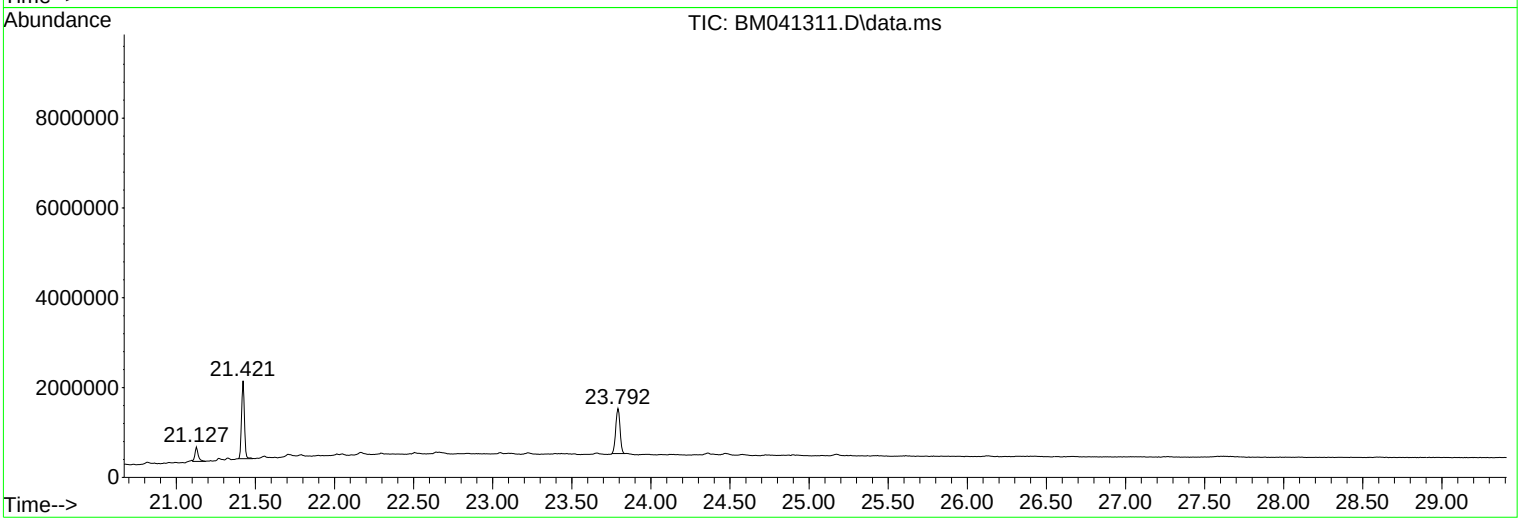
Instrument :
BNA_M
ClientSampleId :
MW-08W

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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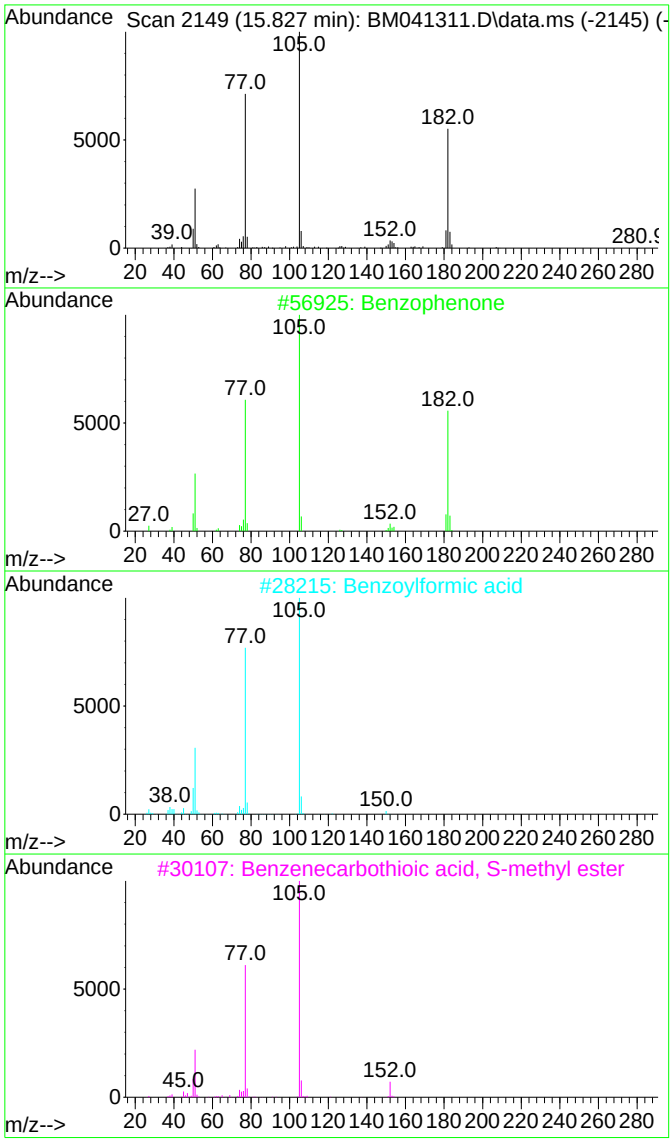
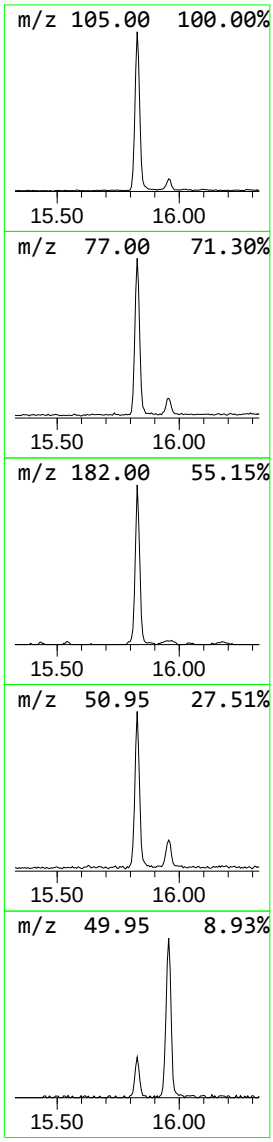
Peak Number 1 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.827	2.53 ng	210279	Acenaphthene-d10	14.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzoylformic acid	150	C8H6O3	000611-73-4	53
3	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	50
4	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	49
5	N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47





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Data File : BM041311.D
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Operator : MA/JU
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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.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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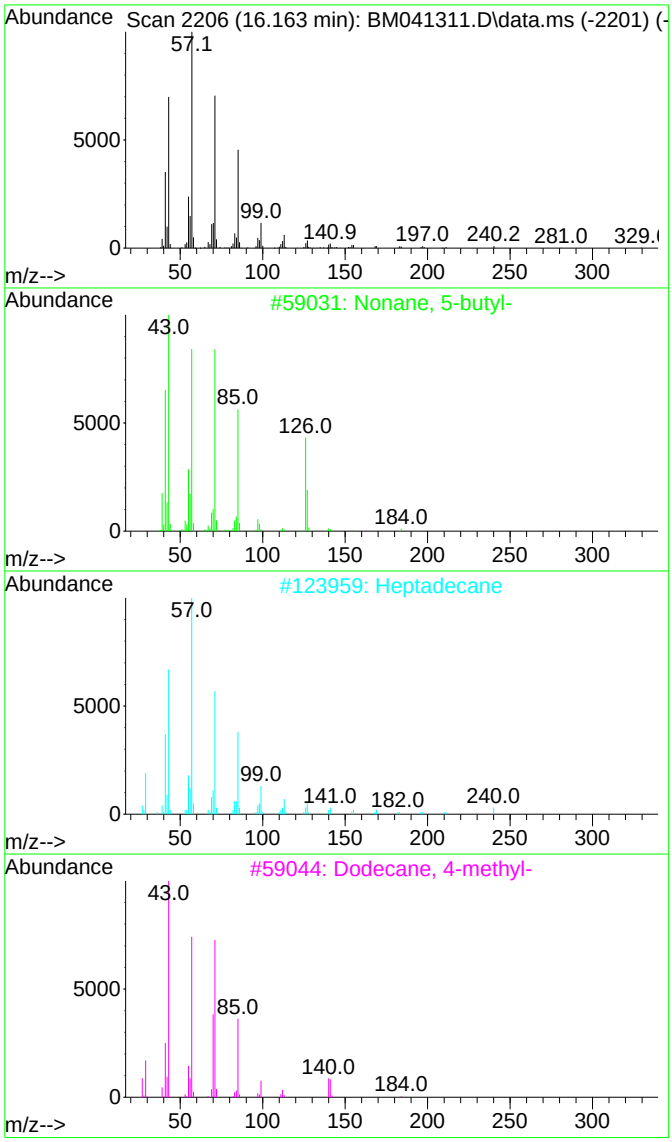
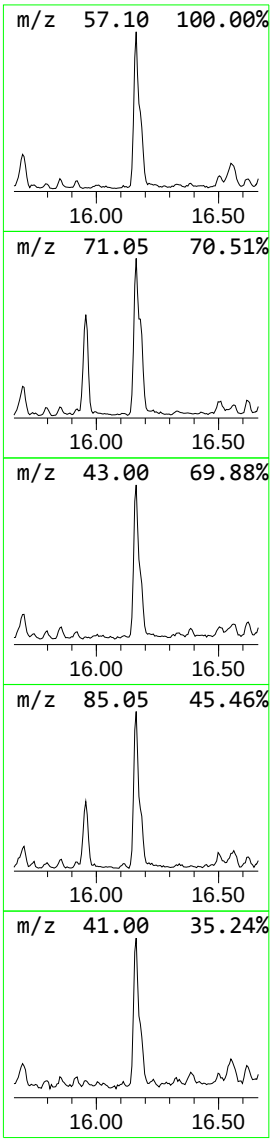
Peak Number 2 Nonane, 5-butyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.163	3.61 ng	387708	Phenanthrene-d10	17.215

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 5-butyl-	184	C13H28	017312-63-9	94
2	Heptadecane	240	C17H36	000629-78-7	93
3	Dodecane, 4-methyl-	184	C13H28	006117-97-1	90
4	Decane, 5-propyl-	184	C13H28	017312-62-8	90
5	Heneicosane	296	C21H44	000629-94-7	90





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Data File : BM041311.D
Acq On : 07 Aug 2023 14:20
Operator : MA/JU
Sample : 03903-18
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-08W

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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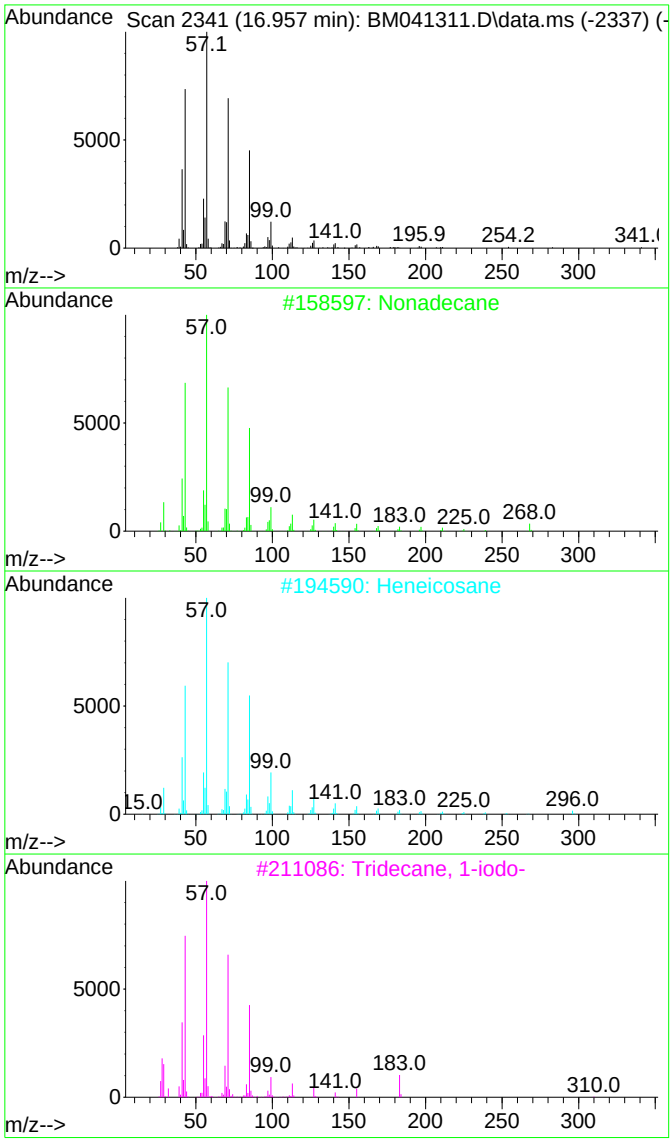
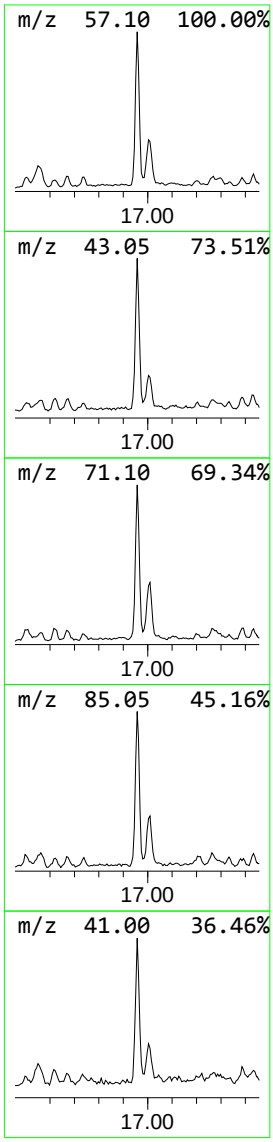
Peak Number 3 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.957	2.37 ng	254166	Phenanthrene-d10	17.215

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	91
2	Heneicosane	296	C21H44	000629-94-7	90
3	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86
4	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	86
5	Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080723\
Data File : BM041311.D
Acq On : 07 Aug 2023 14:20
Operator : MA/JU
Sample : 03903-18
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-08W

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.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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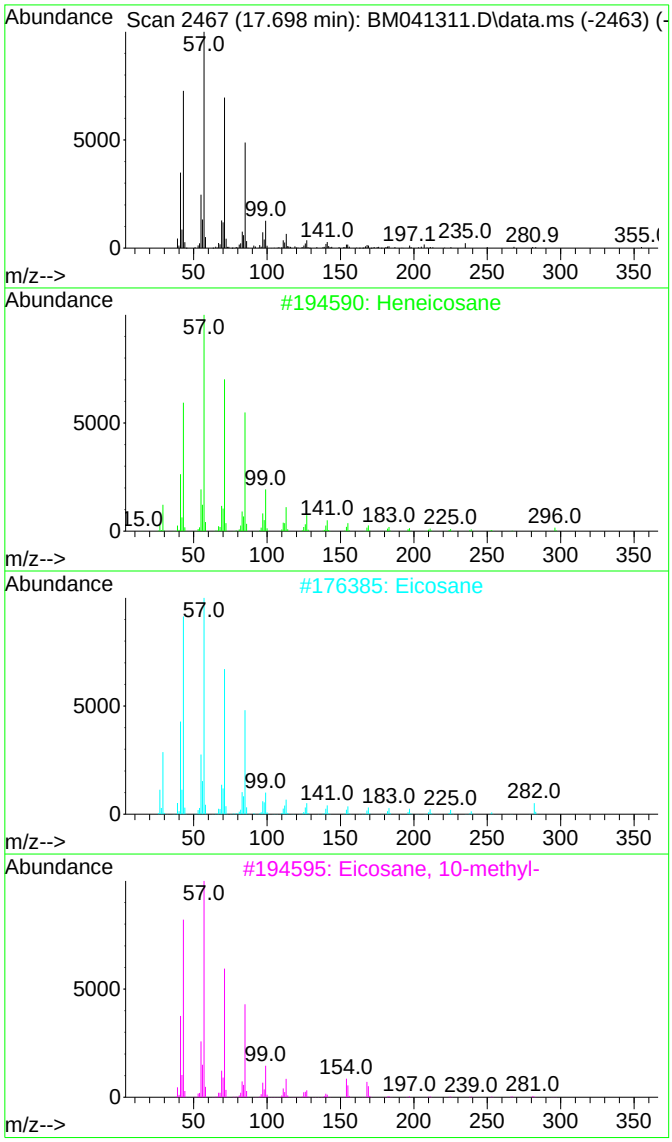
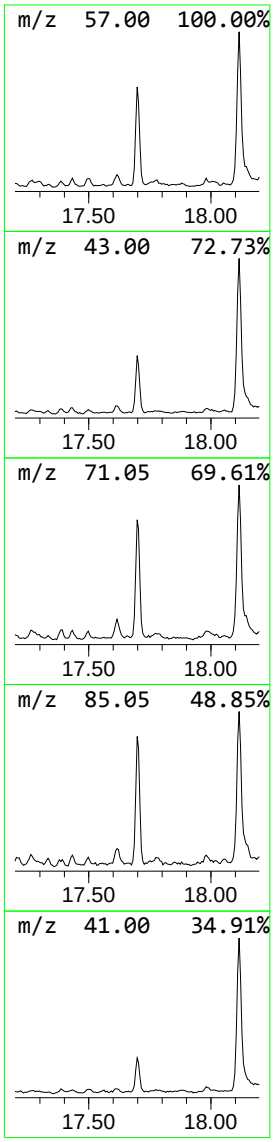
Peak Number 4 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.698	2.29 ng	245548	Phenanthrene-d10	17.215

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Eicosane	282	C20H42	000112-95-8	90
3	Eicosane, 10-methyl-	296	C21H44	054833-23-7	90
4	Heptadecane	240	C17H36	000629-78-7	90
5	Pentadecane	212	C15H32	000629-62-9	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080723\
Data File : BM041311.D
Acq On : 07 Aug 2023 14:20
Operator : MA/JU
Sample : 03903-18
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-08W

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.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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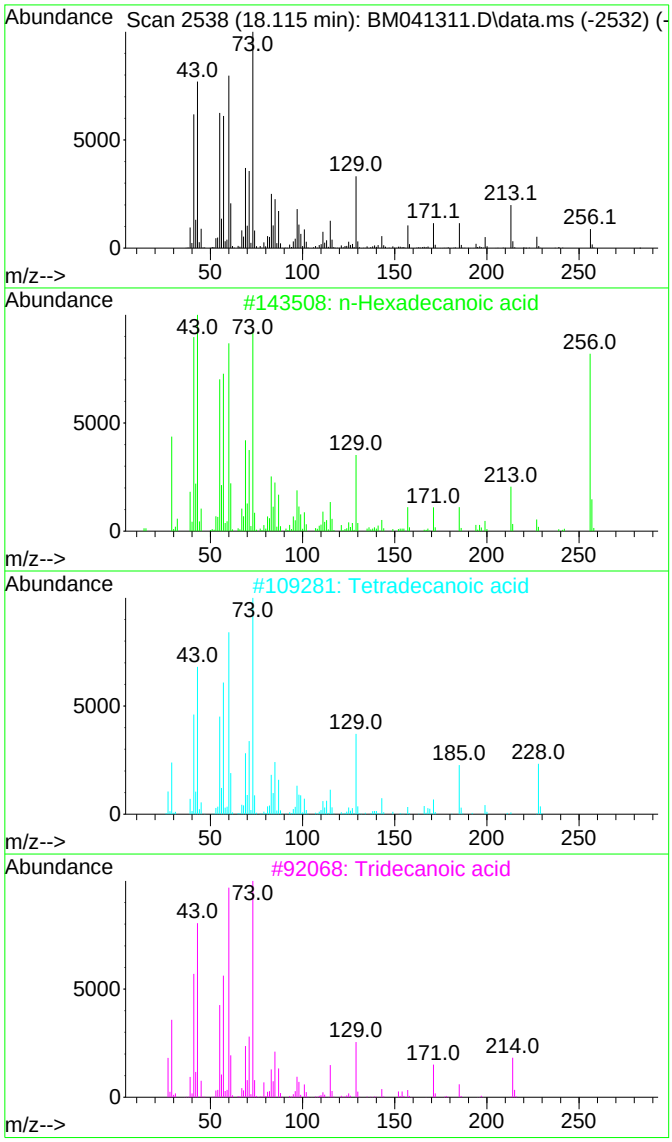
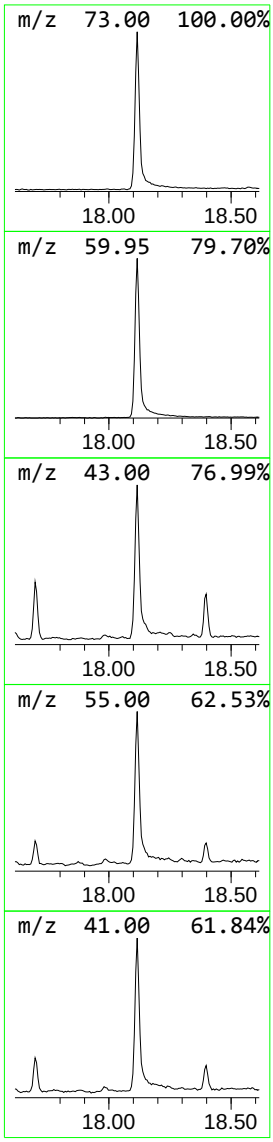
Peak Number 5 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.115	13.45 ng	1444120	Phenanthrene-d10	17.215

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	94
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	Dodecanoic acid	200	C12H24O2	000143-07-7	70





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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-08W

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.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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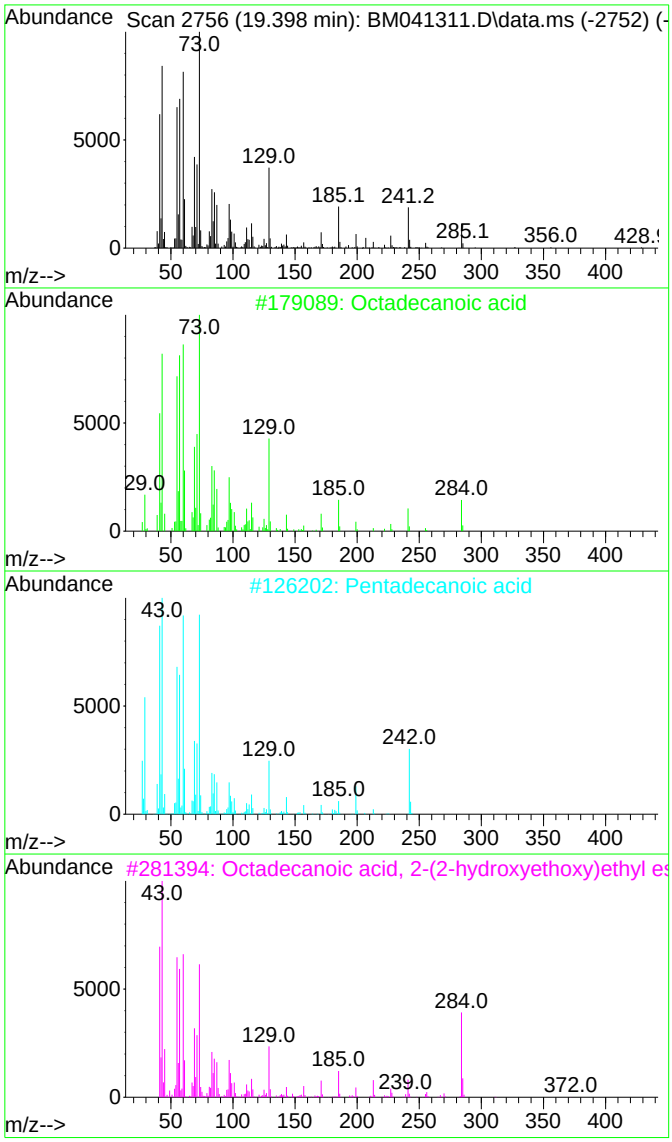
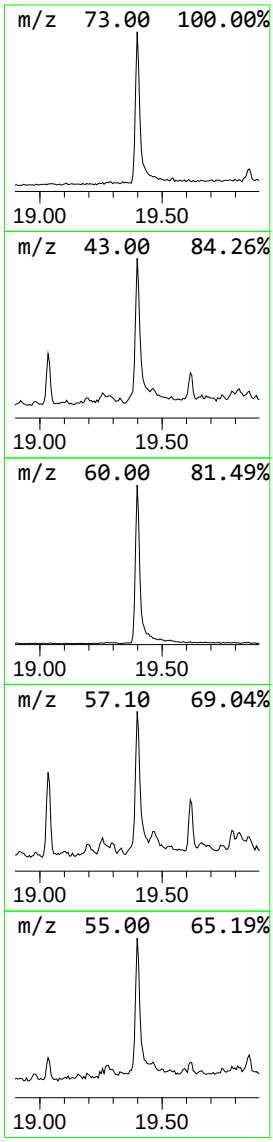
Peak Number 6 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.398	6.84 ng	744448	Chrysene-d12	21.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	60





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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.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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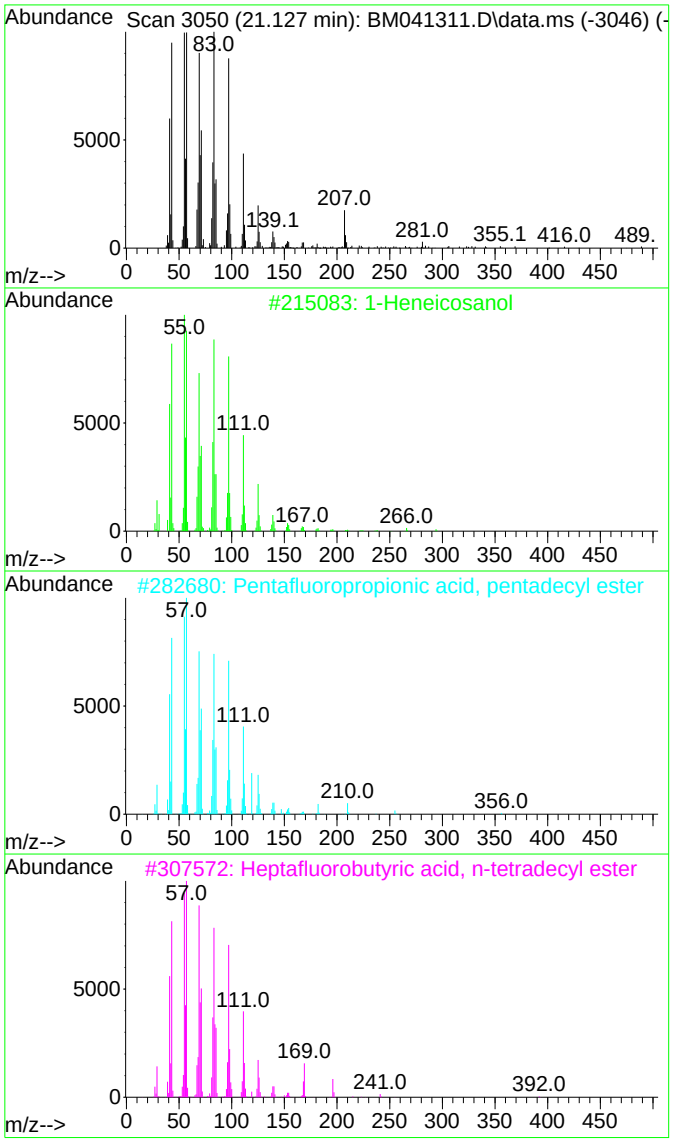
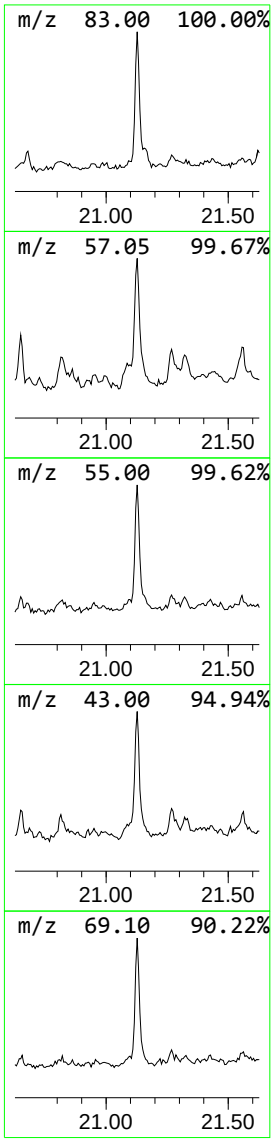
Peak Number 7 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.127	4.20 ng	457042	Chrysene-d12	21.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	94
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
3	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5	Pentacos-1-ene	350	C25H50	016980-85-1	94





Tentatively Identified Compound (LSC) summary

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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
Benzophenone	15.827	2.5	ng	210279	3	14.457	1664590	20.0
Nonane, 5-butyl-	16.163	3.6	ng	387708	4	17.215	2147930	20.0
Nonadecane	16.957	2.4	ng	254166	4	17.215	2147930	20.0
Heneicosane	17.698	2.3	ng	245548	4	17.215	2147930	20.0
n-Hexadecanoic ...	18.115	13.4	ng	1444120	4	17.215	2147930	20.0
Octadecanoic acid	19.398	6.8	ng	744448	5	21.421	2175560	20.0
1-Heneicosanol	21.127	4.2	ng	457042	5	21.421	2175560	20.0