LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080422\
Data File : BM036107.D
Acq On : 04 Aug 2022 20:21
Operator : CG/JU
Sample : N3931-17
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RVE-128

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-BM080122.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM036107.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.428	391	398	411	rBV	5134038	7262179	43.36%	7.196%
2	7.040	660	672	685	rBV	5068124	7957493	47.51%	7.885%
3	7.857	804	811	819	rBV	1203973	1881532	11.23%	1.864%
4	9.028	1003	1010	1025	rBV	3152090	5205626	31.08%	5.158%
5	10.669	1280	1289	1300	rBV	1719167	2908271	17.36%	2.882%
6	13.128	1699	1707	1717	rBV	8554151	12510626	74.69%	12.396%
7	14.504	1934	1941	1958	rVB	2721139	4039700	24.12%	4.003%
8	15.986	2187	2193	2203	rBV	7180151	10661175	63.65%	10.564%
9	17.245	2398	2407	2411	rBV	3247457	4737129	28.28%	4.694%
10	17.286	2411	2414	2418	rVB	207180	256853	1.53%	0.255%
11	18.139	2554	2559	2569	rBV2	347070	544990	3.25%	0.540%
12	19.298	2752	2756	2762	rBV	262113	343127	2.05%	0.340%
13	19.662	2813	2818	2826	rVB2	215174	378105	2.26%	0.375%
14	19.868	2847	2853	2858	rBV	14047168	16749110	100.00%	16.596%
15	20.156	2898	2902	2904	rBV	180032	254358	1.52%	0.252%
16	20.598	2974	2977	2981	rBV	151265	234886	1.40%	0.233%
17	20.851	3017	3020	3024	rBV2	150939	188060	1.12%	0.186%
18	21.139	3065	3069	3077	rBV	1833992	2339840	13.97%	2.318%
19	21.421	3112	3117	3122	rBV	3101525	4024900	24.03%	3.988%
20	22.033	3218	3221	3223	rBV	439754	534040	3.19%	0.529%
21	23.068	3393	3397	3402	rBV	549343	817176	4.88%	0.810%
22	23.786	3513	3519	3529	rVB2	1678098	3376702	20.16%	3.346%
23	24.397	3619	3623	3632	rVB	724391	1431301	8.55%	1.418%
24	24.503	3636	3641	3653	rVB	726515	1869162	11.16%	1.852%
25	26.497	3971	3980	3997	rVB	3345768	10416774	62.19%	10.321%

Sum of corrected areas: 100923115

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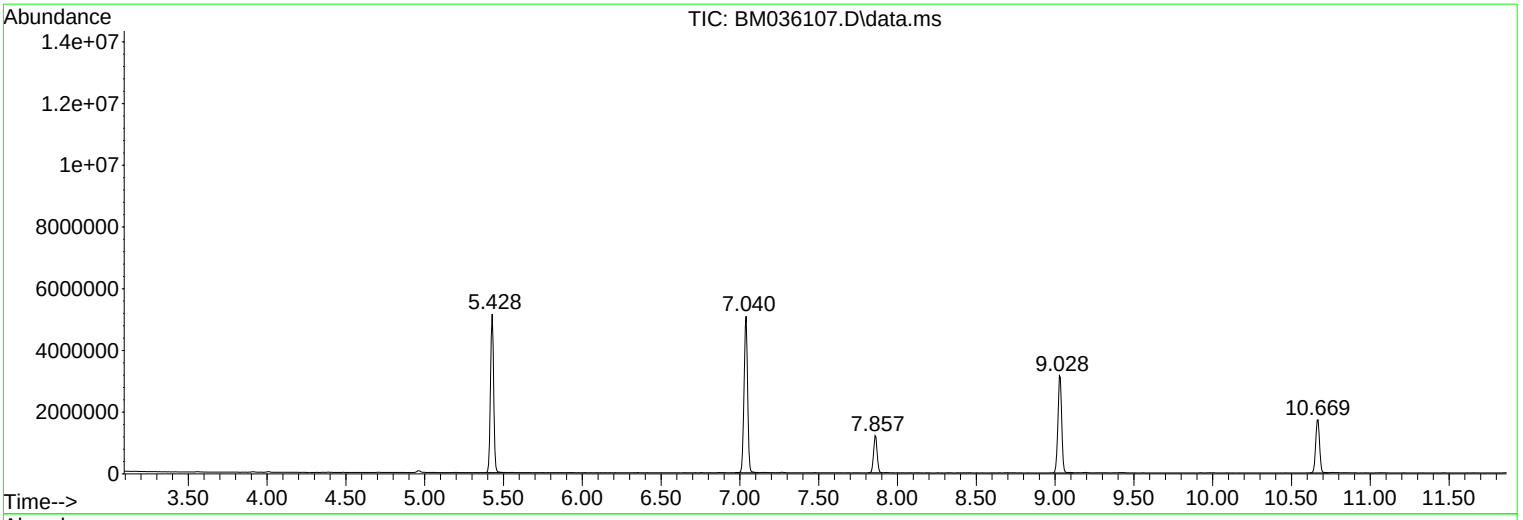
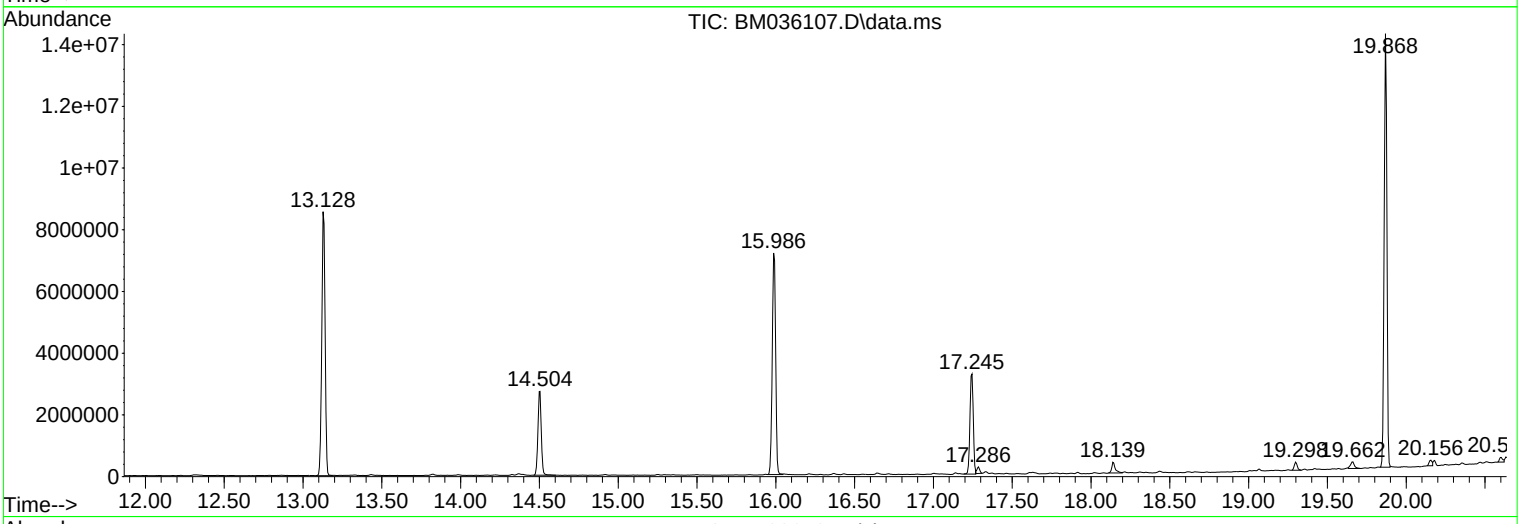
ALS Vial : 16 Sample Multiplier: 1

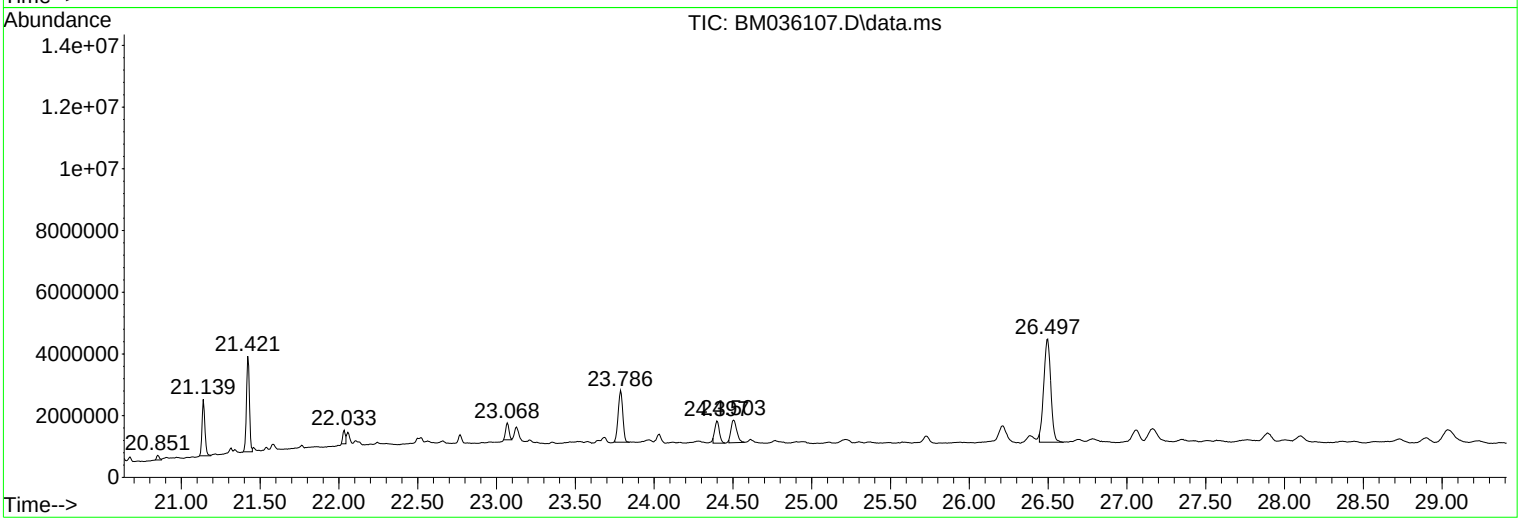
Instrument :
BNA_M
ClientSampleId :
RVE-128

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.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 : BM036107.D
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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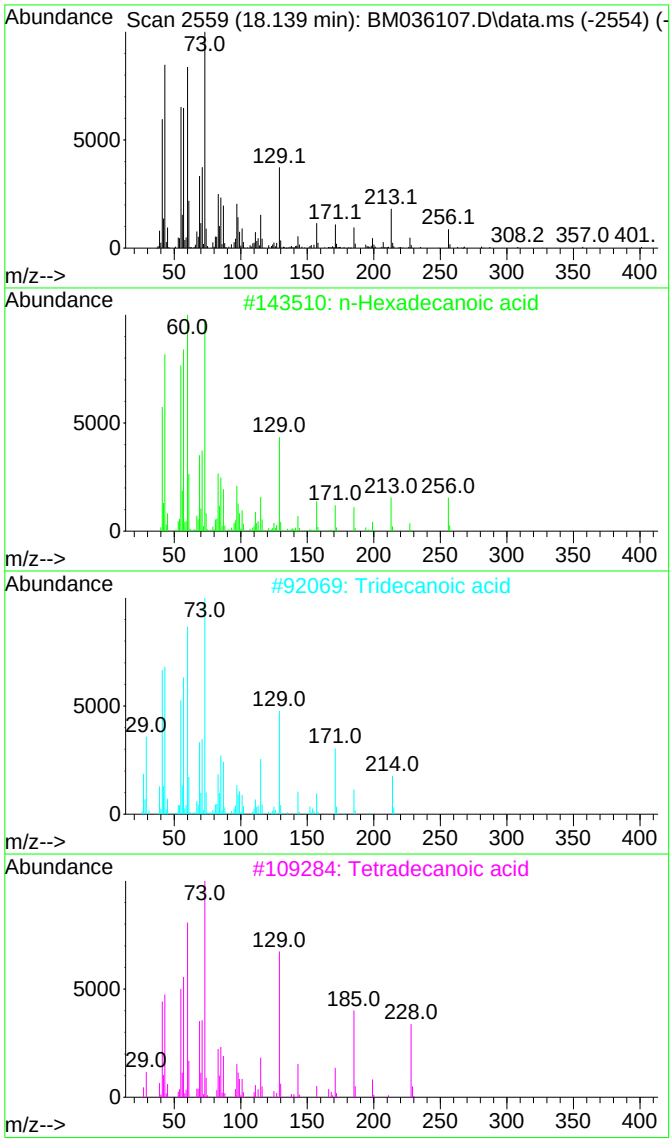
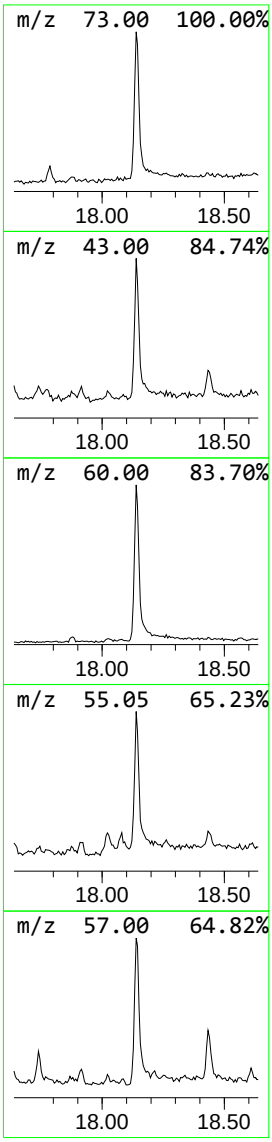
Peak Number 1 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.139	2.30 ng	544990	Phenanthrene-d10	17.245

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	94
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5	Octadecanoic acid	284	C18H36O2	000057-11-4	81





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Data File : BM036107.D
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Operator : CG/JU
Sample : N3931-17
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RVE-128

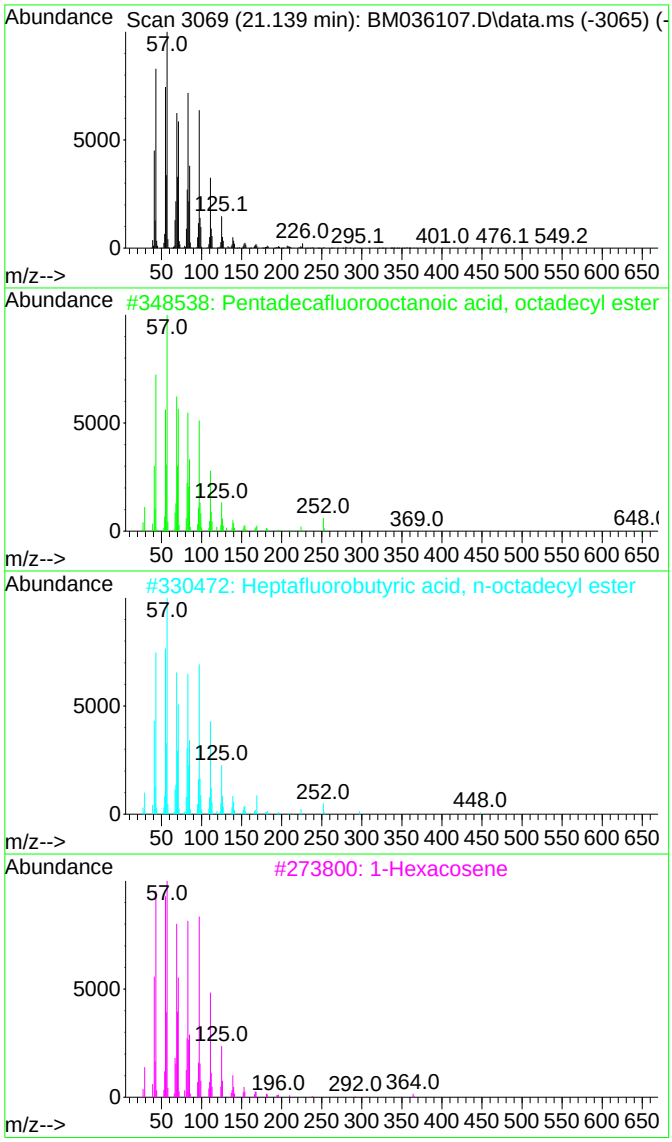
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

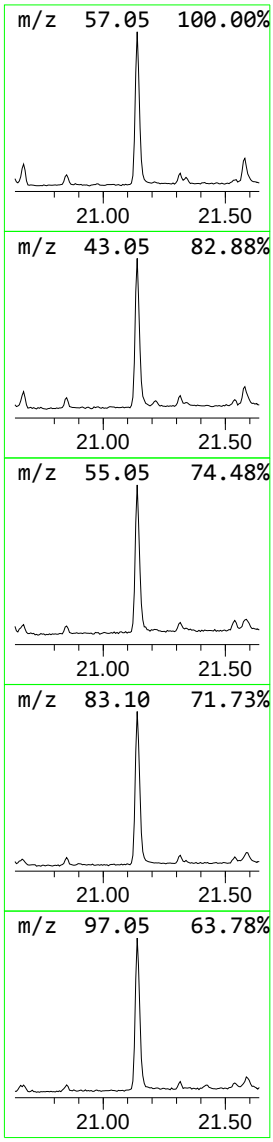
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Pentadecafluorooctanoic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.139	11.63 ng	2339840	Chrysene-d12	21.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
3	1-Hexacosene	364	C26H52	018835-33-1	91
4	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
5	17-Pentatriacontene	491	C35H70	006971-40-0	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080422\
Data File : BM036107.D
Acq On : 04 Aug 2022 20:21
Operator : CG/JU
Sample : N3931-17
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RVE-128

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.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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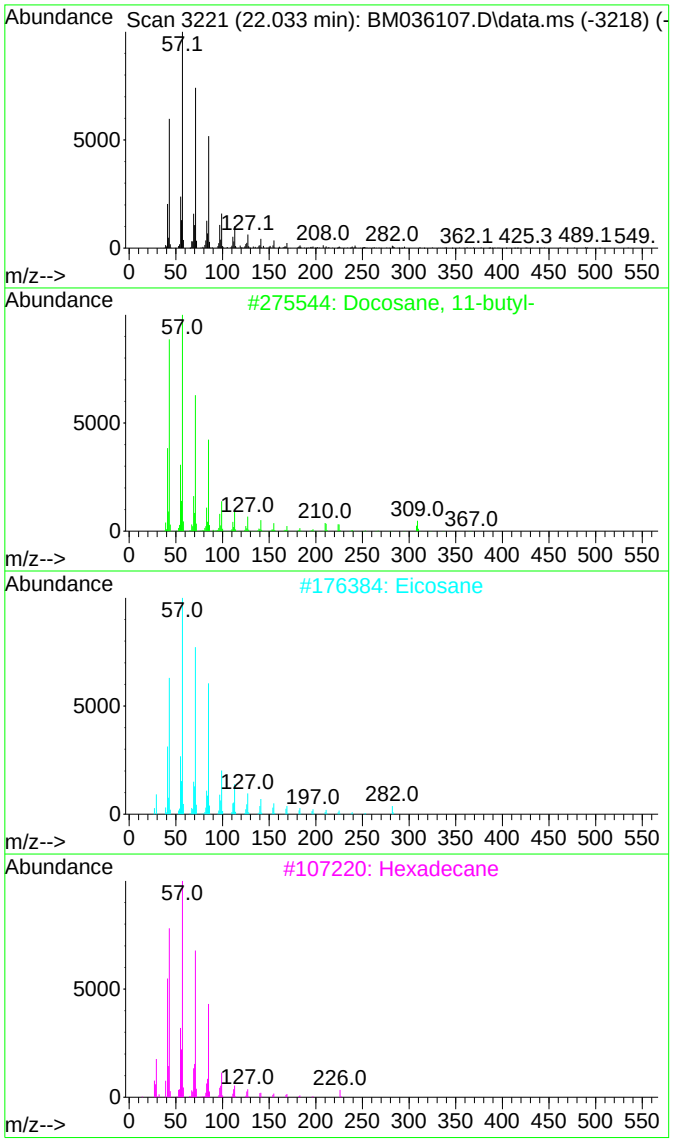
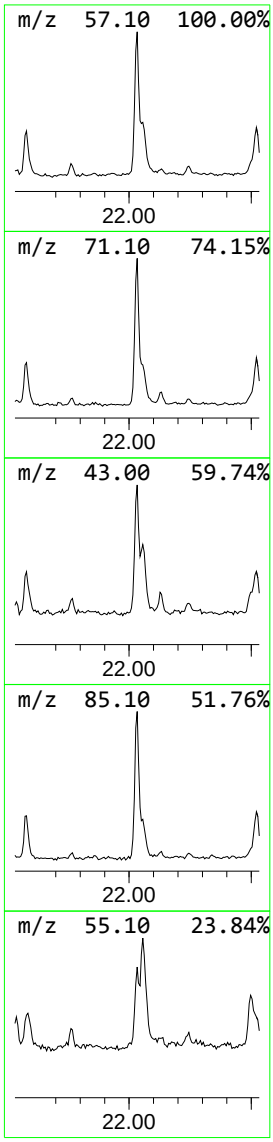
Peak Number 3 Docosane, 11-butyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.033	2.65 ng	534040	Chrysene-d12	21.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane, 11-butyl-	366	C26H54	013475-76-8	95
2	Eicosane	282	C20H42	000112-95-8	94
3	Hexadecane	226	C16H34	000544-76-3	91
4	Hexatriacontane	507	C36H74	000630-06-8	91
5	Hexacosane	366	C26H54	000630-01-3	91





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Data File : BM036107.D
Acq On : 04 Aug 2022 20:21
Operator : CG/JU
Sample : N3931-17
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RVE-128

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

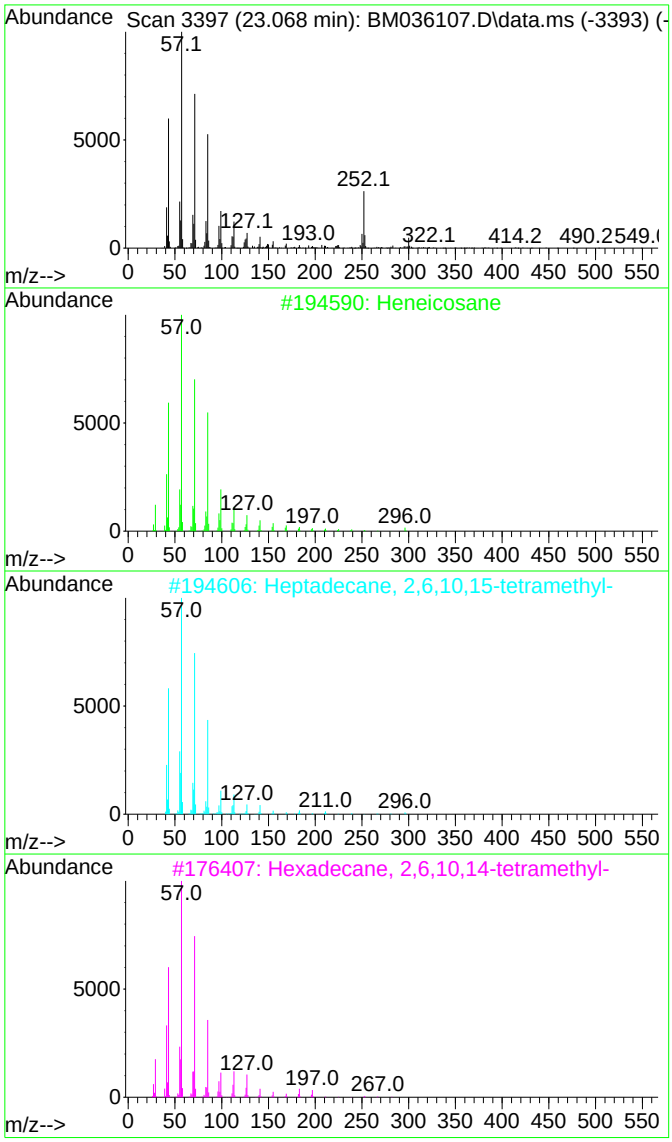
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

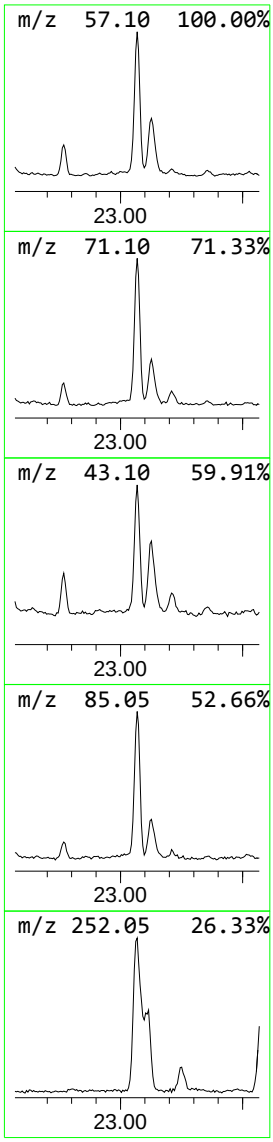
****

Peak Number 4 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.068	4.84 ng	817176	Perylene-d12	23.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	98
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	89
3	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	83
4	Octacosane	394	C28H58	000630-02-4	81
5	Hexacosane	366	C26H54	000630-01-3	81





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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RVE-128

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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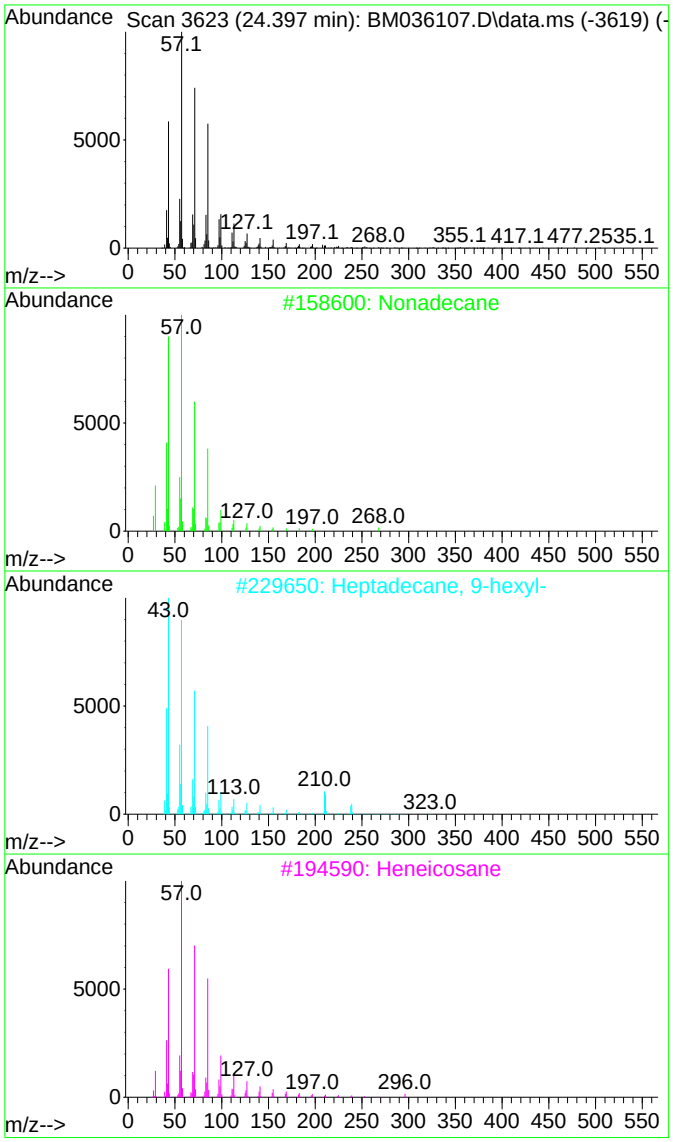
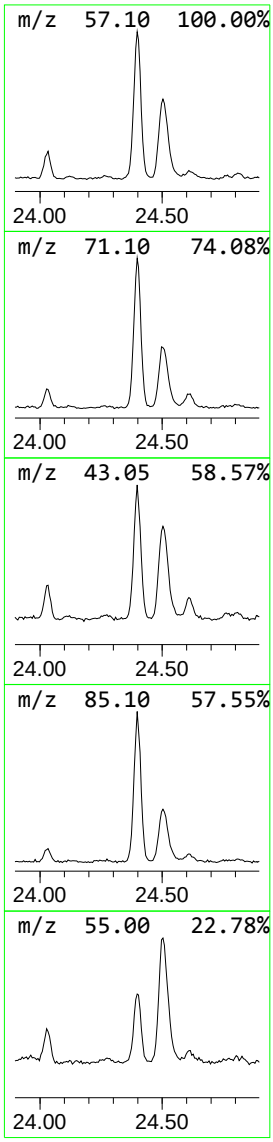
Peak Number 5 Nonadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.397	8.48 ng	1431300	Perylene-d12	23.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	95
2	Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	93
3	Heneicosane	296	C21H44	000629-94-7	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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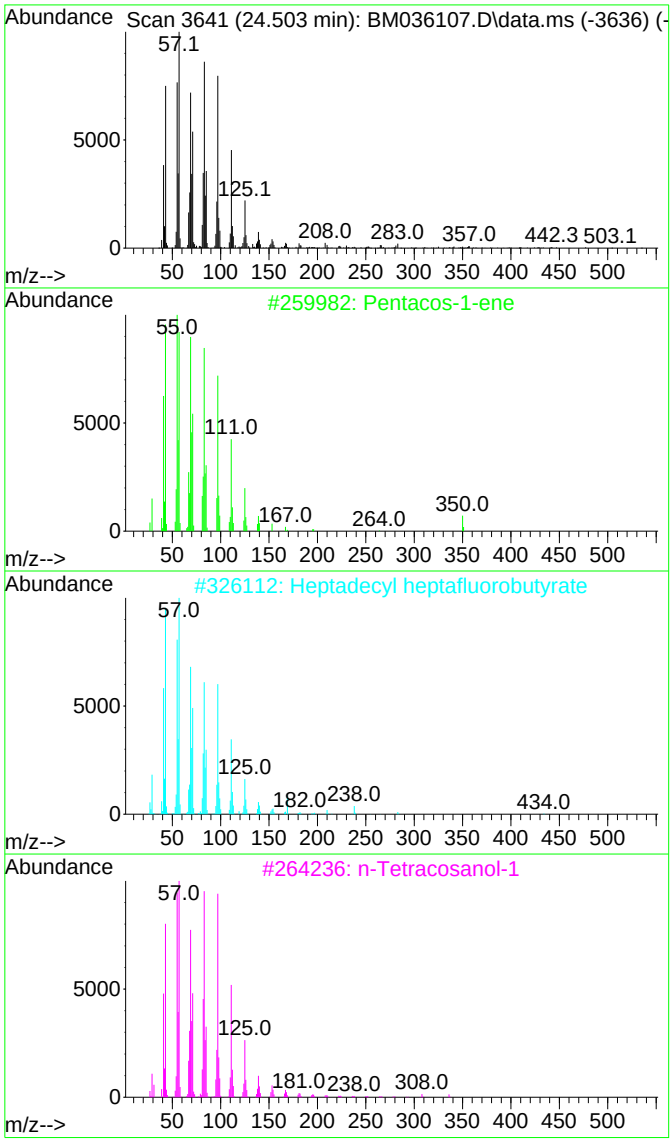
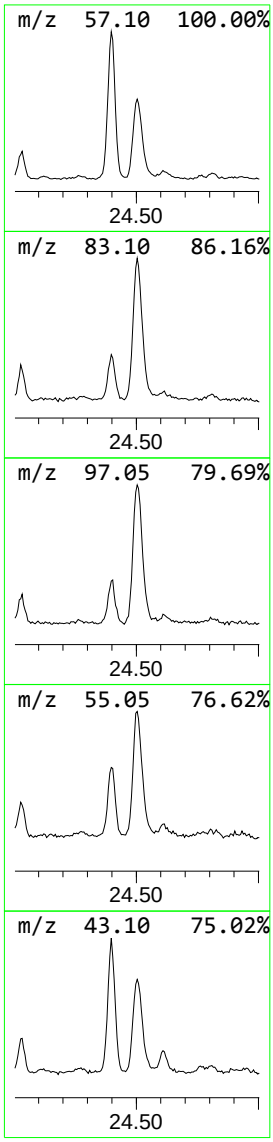
Peak Number 6 Pentacos-1-ene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.503	11.07 ng	1869160	Perylene-d12	23.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacos-1-ene	350	C25H50	016980-85-1	95
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	1-Hexacosene	364	C26H52	018835-33-1	94
5	Behenic alcohol	326	C22H46O	000661-19-8	94





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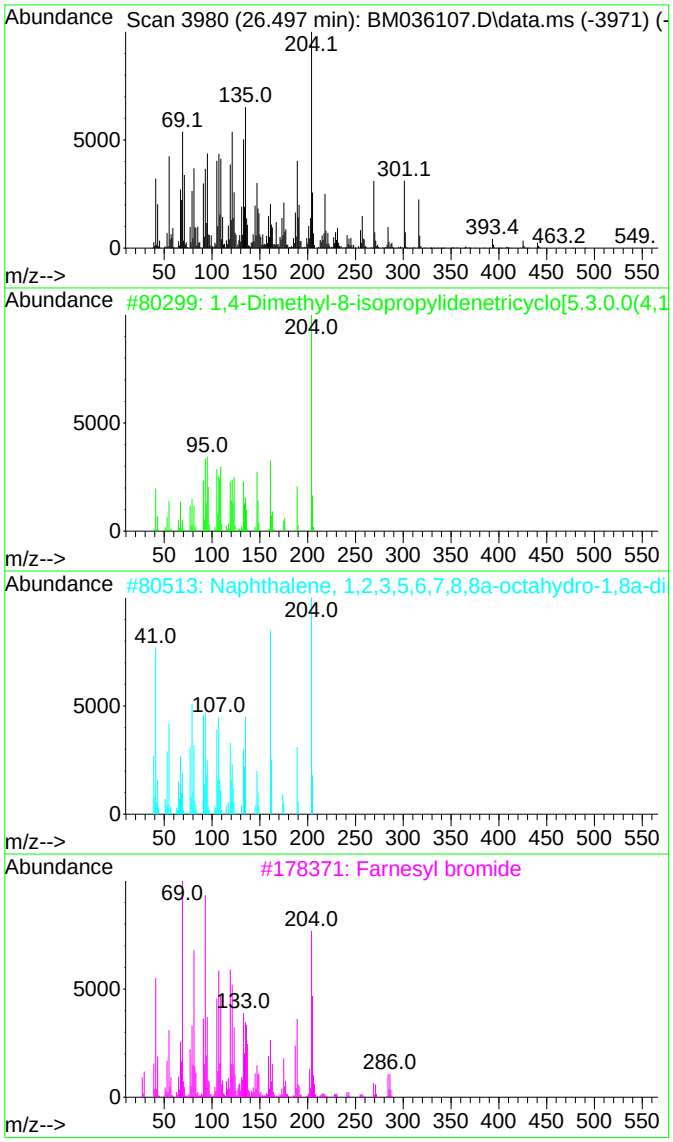
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

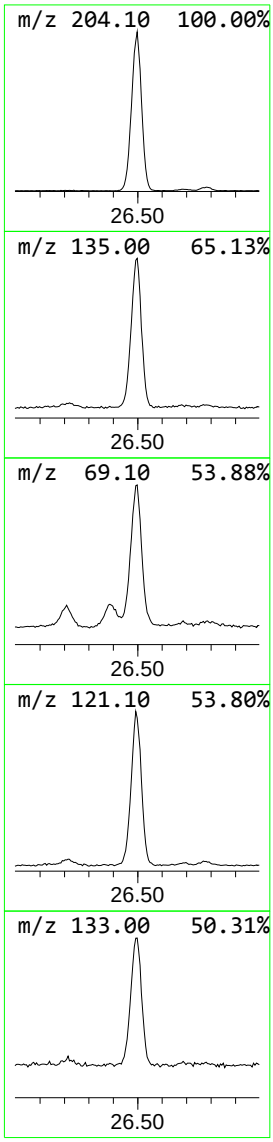
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1,4-Dimethyl-8-isopropylide... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.497	61.70 ng	10416800	Perylene-d12	23.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1010140-07-7	53
2	Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	49
3	Farnesyl bromide	284	C15H25Br	006874-67-5	49
4	2,5,5,8a-Tetramethyl-6,7,8,8a-te...	204	C14H20O	124957-09-1	46
5	1H-3a,7-Methanoazulene, 2,3,6,7,...	204	C15H24	000560-32-7	43





Tentatively Identified Compound (LSC) summary

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Hexadecanoic ...	18.139	2.3	ng	544990	4	17.245	4737130	20.0
Pentadecafluoro...	21.139	11.6	ng	2339840	5	21.421	4024900	20.0
Docosane, 11-bu...	22.033	2.6	ng	534040	5	21.421	4024900	20.0
Heneicosane	23.068	4.8	ng	817176	6	23.786	3376700	20.0
Nonadecane	24.397	8.5	ng	1431300	6	23.786	3376700	20.0
Pentacos-1-ene	24.503	11.1	ng	1869160	6	23.786	3376700	20.0
1,4-Dimethyl-8-...	26.497	61.7	ng	10416800	6	23.786	3376700	20.0