LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010722\
Data File : BM033683.D
Acq On : 07 Jan 2022 23:40
Operator : CG/JU
Sample : N1065-18
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
AMI-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_M\Methods\8270-BM010522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM033683.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.043	302	307	313	rVB2	67030	96174	1.06%	0.212%
2	5.519	381	388	398	rVB	2362269	3407375	37.73%	7.497%
3	7.131	653	662	674	rBV	2346427	3726975	41.27%	8.200%
4	7.972	798	805	813	rVB	583955	942397	10.44%	2.073%
5	9.136	993	1003	1015	rBV	1520590	2473878	27.39%	5.443%
6	10.566	1240	1246	1253	rBV	143954	221942	2.46%	0.488%
7	10.789	1275	1284	1292	rBV	804961	1368427	15.15%	3.011%
8	13.242	1694	1701	1711	rBV	3874937	5629953	62.34%	12.387%
9	14.613	1927	1934	1943	rBV	1326696	1915303	21.21%	4.214%
10	16.089	2179	2185	2204	rBV	3186797	4824363	53.42%	10.615%
11	17.348	2392	2399	2404	rBV	1690012	2422107	26.82%	5.329%
12	18.242	2545	2551	2554	rBV3	110457	159129	1.76%	0.350%
13	19.395	2743	2747	2754	rVB	95186	120386	1.33%	0.265%
14	19.753	2804	2808	2817	rVB	123662	197181	2.18%	0.434%
15	19.959	2837	2843	2855	rVB	7163292	9031079	100.00%	19.870%
16	21.224	3054	3058	3064	rBV2	285362	368868	4.08%	0.812%
17	21.430	3089	3093	3100	rVB	551751	616956	6.83%	1.357%
18	21.512	3101	3107	3111	rBV	2149183	2944614	32.61%	6.479%
19	21.677	3132	3135	3138	rBV	87152	99122	1.10%	0.218%
20	22.141	3211	3214	3220	rVB2	145239	199605	2.21%	0.439%
21	22.647	3296	3300	3309	rVB	177114	277711	3.08%	0.611%
22	23.206	3392	3395	3406	rVB2	266330	485190	5.37%	1.068%
23	23.847	3501	3504	3511	rVB	293700	500112	5.54%	1.100%
24	23.930	3511	3518	3536	rVB2	1313514	2844749	31.50%	6.259%
25	24.588	3626	3630	3637	rVB	284176	576157	6.38%	1.268%

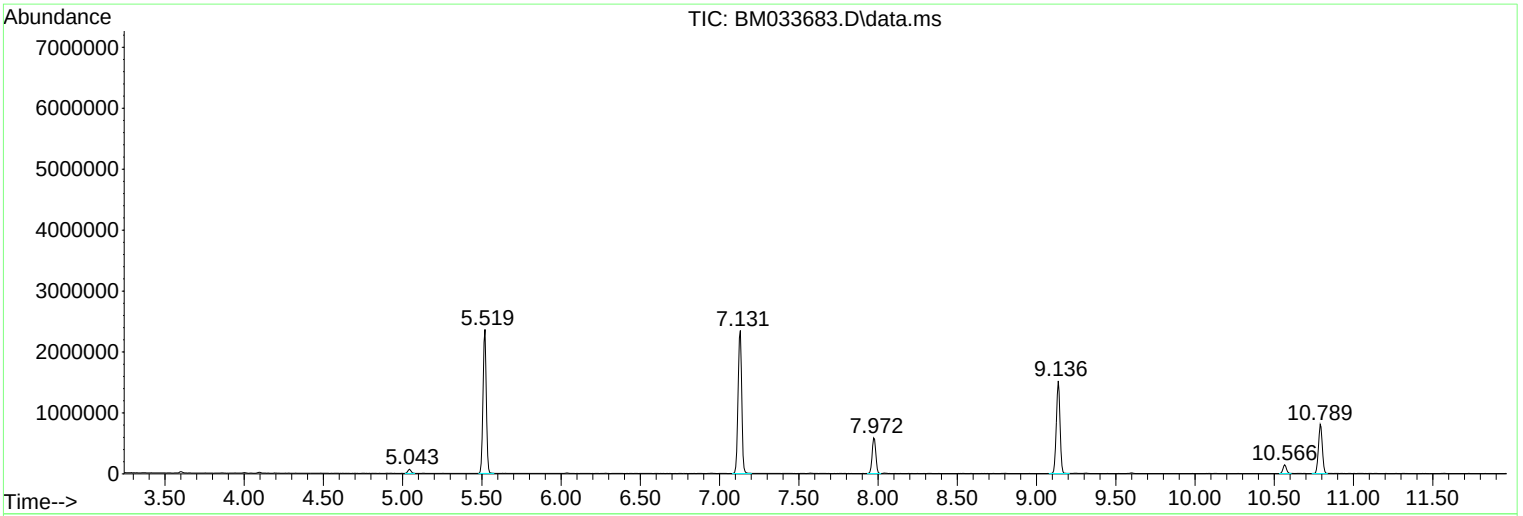
Sum of corrected areas: 45449753

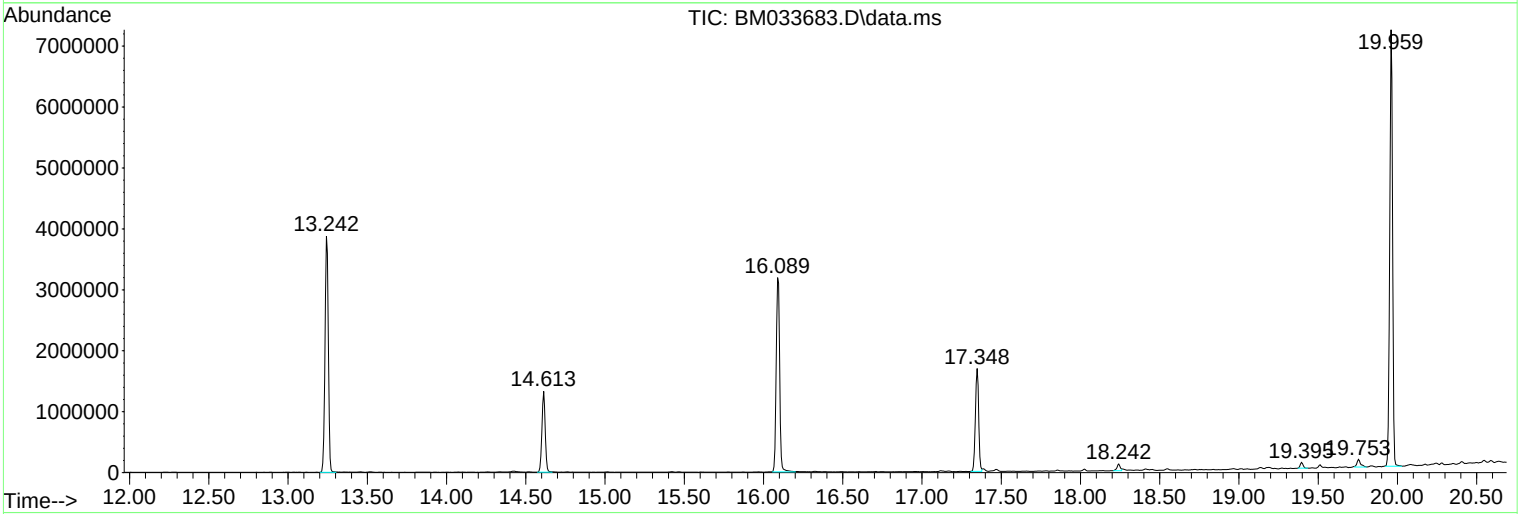
Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010722\
Data File : BM033683.D
Acq On : 07 Jan 2022 23:40
Operator : CG/JU
Sample : N1065-18
Misc :
ALS Vial : 18 Sample Multiplier: 1

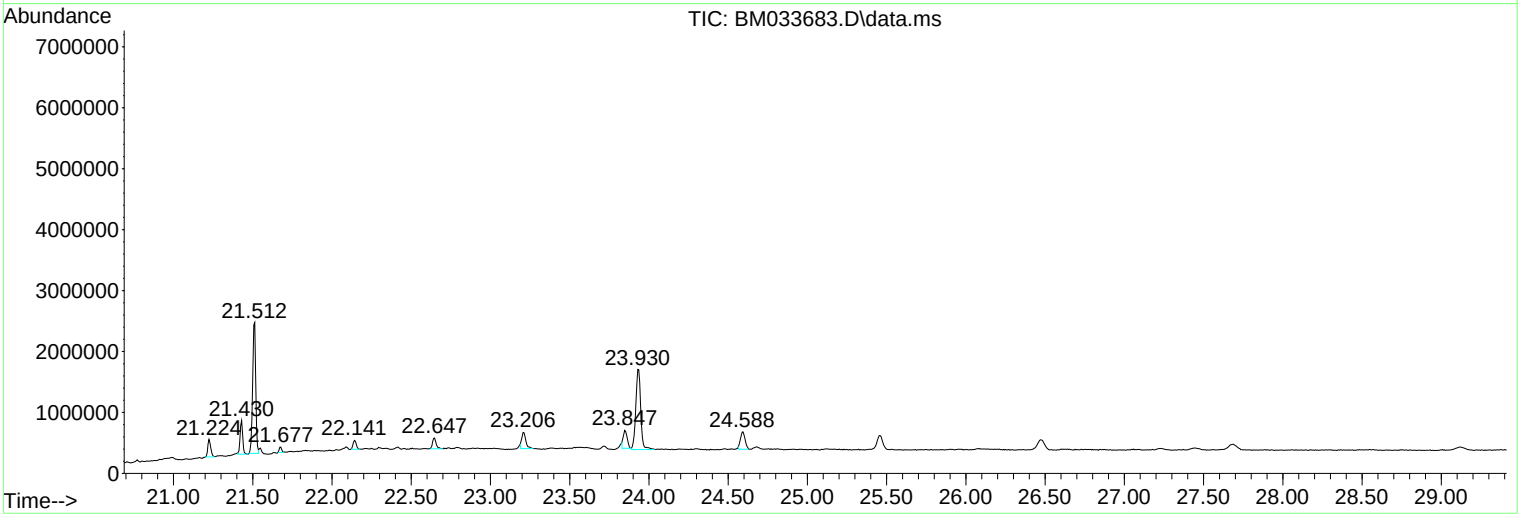
Instrument :
BNA_M
ClientSampleId :
AMI-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM010522.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\BM010722\
Data File : BM033683.D
Acq On : 07 Jan 2022 23:40
Operator : CG/JU
Sample : N1065-18
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
AMI-5

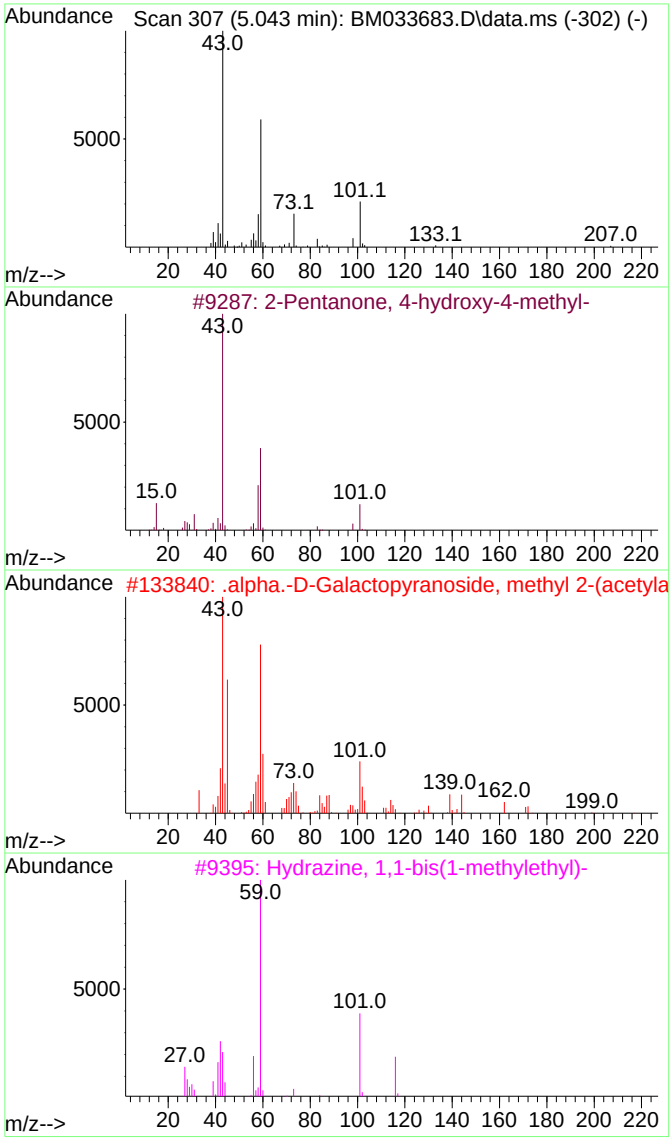
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM010522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

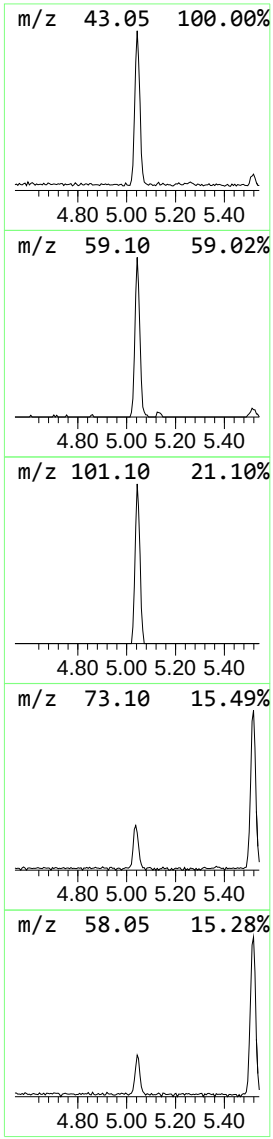
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.043	2.04 ng	96174	1,4-Dichlorobenzene-d4	7.972

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	.alpha.-D-Galactopyranoside, met...	249	C10H19NO6	017296-07-0	39
3	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	37
4	3-Octanol	130	C8H18O	000589-98-0	28
5	4-Ethyl-3-octanol	158	C10H22O	019781-26-1	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010722\
Data File : BM033683.D
Acq On : 07 Jan 2022 23:40
Operator : CG/JU
Sample : N1065-18
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
AMI-5

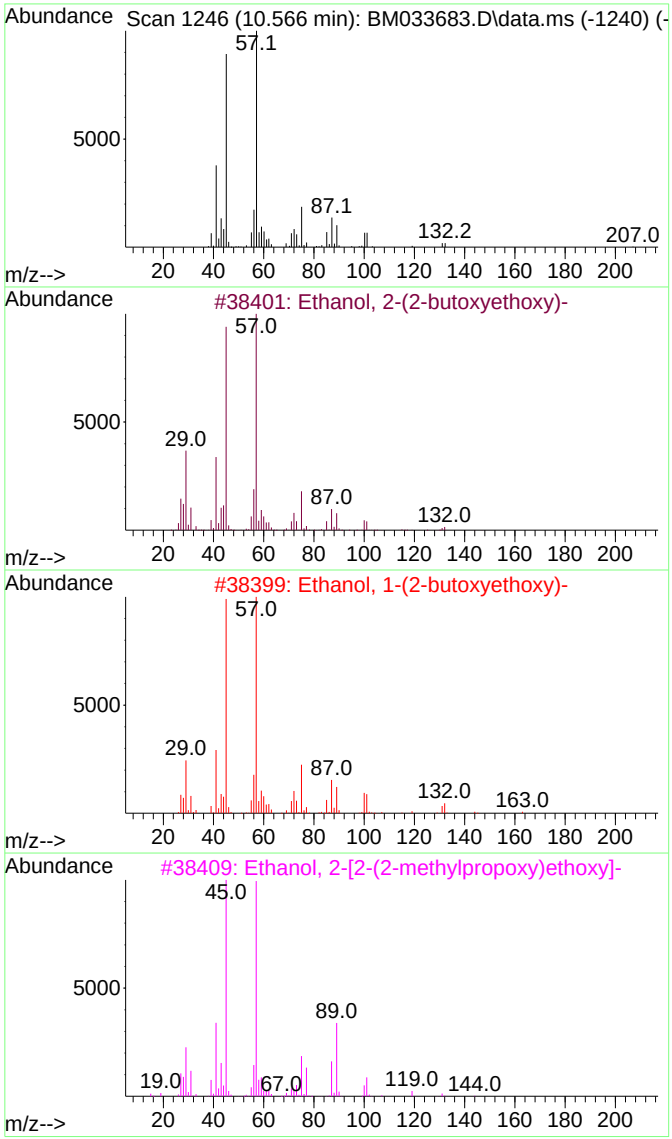
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM010522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

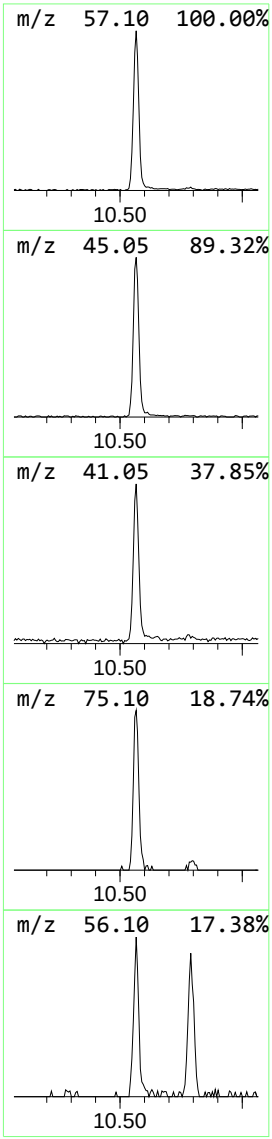
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.566	3.24 ng	221942	Naphthalene-d8	10.789

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	78
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
5	Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010722\
Data File : BM033683.D
Acq On : 07 Jan 2022 23:40
Operator : CG/JU
Sample : N1065-18
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
AMI-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM010522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

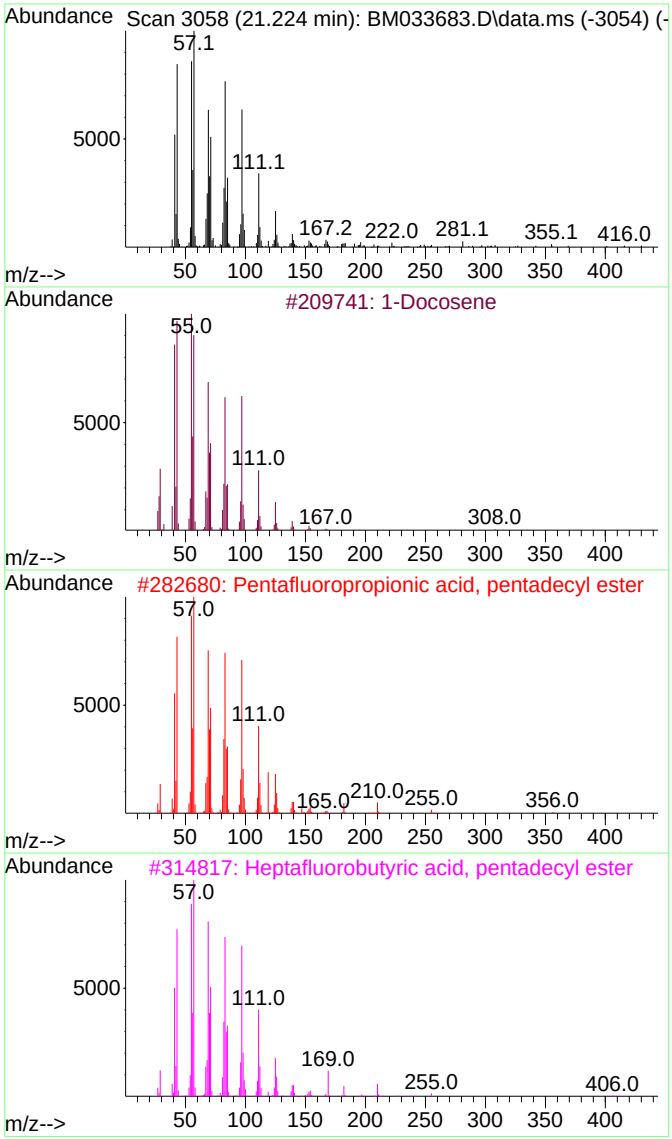
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

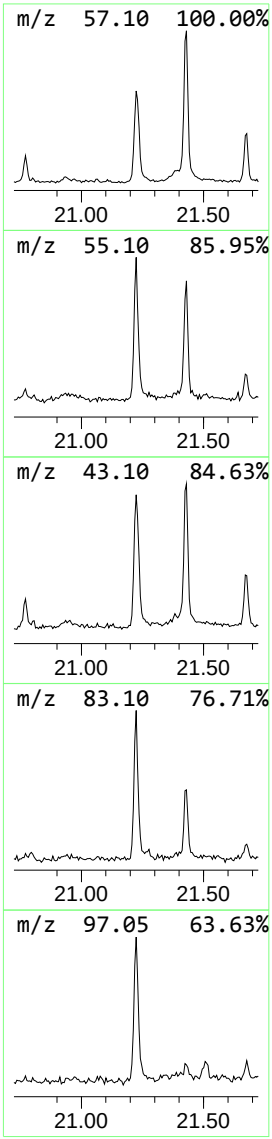
****

Peak Number 3 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.224	2.51 ng	368868	Chrysene-d12	21.512

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	97
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
4	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010722\
Data File : BM033683.D
Acq On : 07 Jan 2022 23:40
Operator : CG/JU
Sample : N1065-18
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
AMI-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM010522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

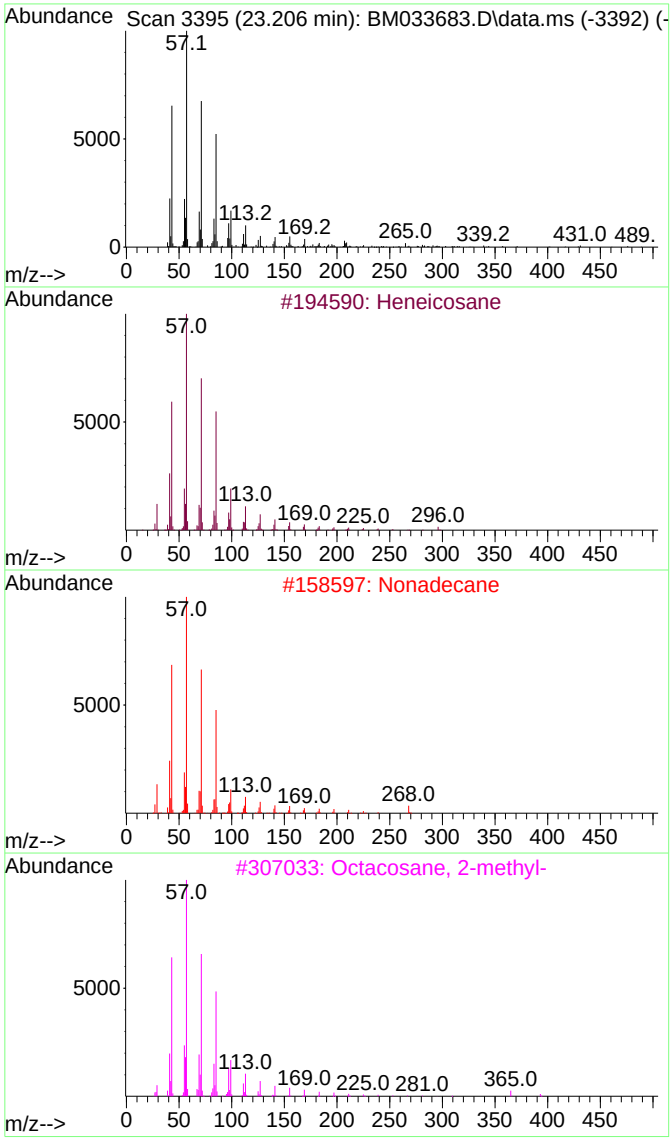
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

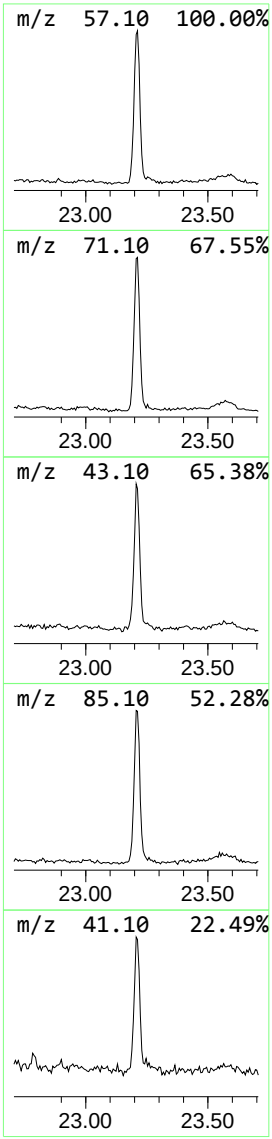
****

Peak Number 4 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.206	3.41 ng	485190	Perylene-d12	23.936

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	87
2	Nonadecane	268	C19H40	000629-92-5	87
3	Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5	Docosane, 1-iodo-	436	C22H45I	1000406-31-9	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010722\
Data File : BM033683.D
Acq On : 07 Jan 2022 23:40
Operator : CG/JU
Sample : N1065-18
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
AMI-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM010522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

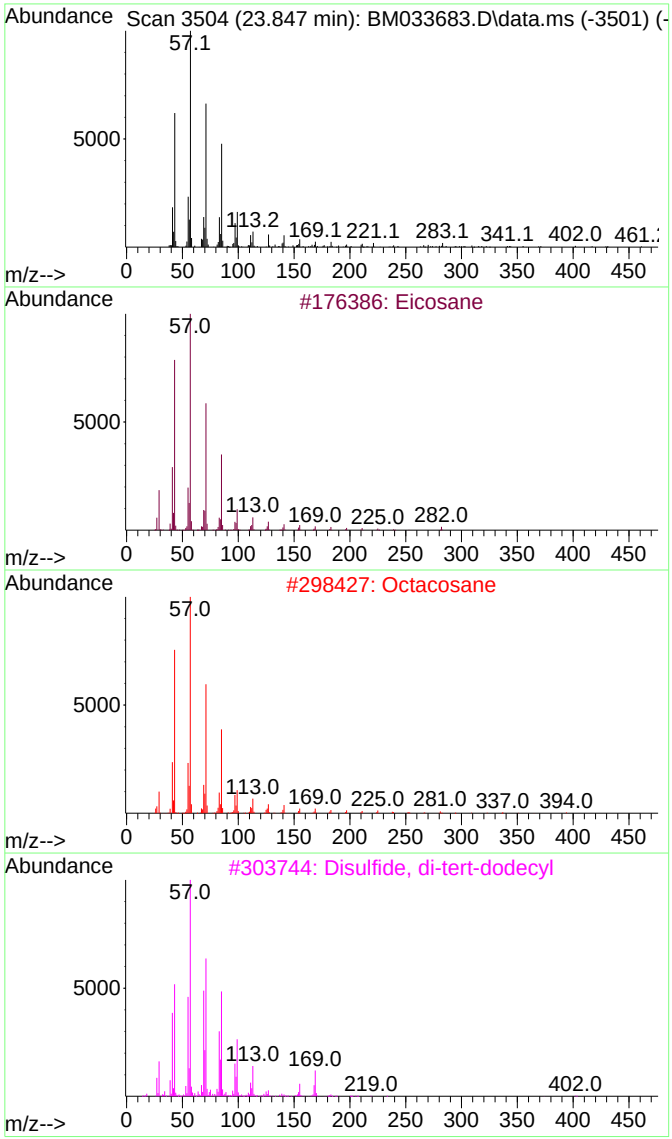
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

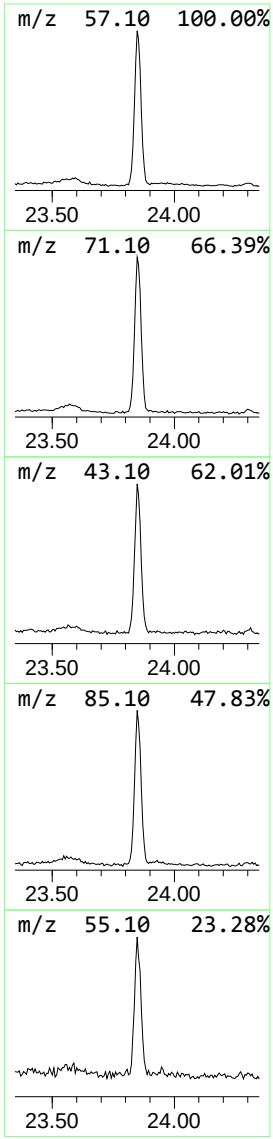
****

Peak Number 5 Eicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.847	3.52 ng	500112	Perylene-d12	23.936

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Octacosane	394	C28H58	000630-02-4	90
3	Disulfide, di-tert-dodecyl	402	C24H50S2	027458-90-8	90
4	Tetracosane	338	C24H50	000646-31-1	90
5	Heptacosane	380	C27H56	000593-49-7	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010722\
Data File : BM033683.D
Acq On : 07 Jan 2022 23:40
Operator : CG/JU
Sample : N1065-18
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
AMI-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM010522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

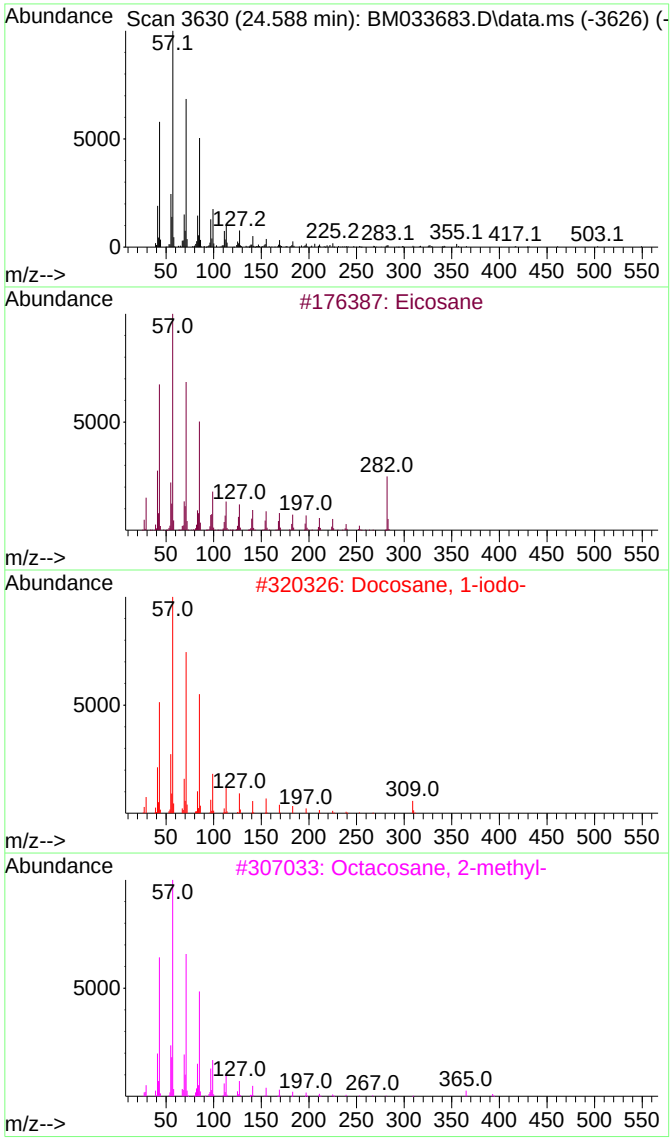
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

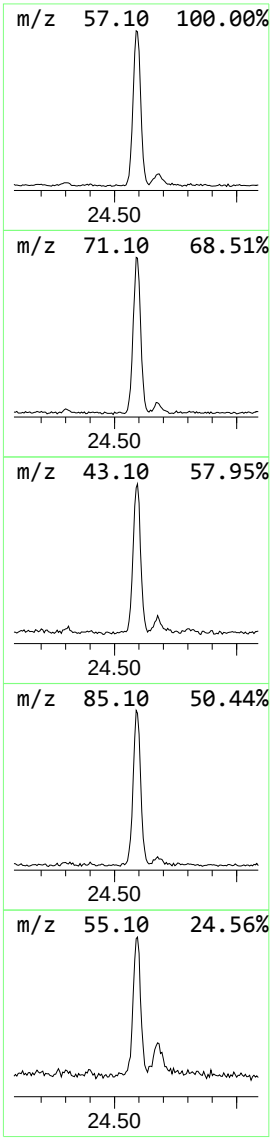
****

Peak Number 6 Docosane, 1-iodo- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.588	4.05 ng	576157	Perylene-d12	23.936

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Docosane, 1-iodo-	436	C22H45I	1000406-31-9	90
3	Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010722\
Data File : BM033683.D
Acq On : 07 Jan 2022 23:40
Operator : CG/JU
Sample : N1065-18
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
AMI-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM010522.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
2-Pentanone, 4-...	5.043	2.0	ng	96174	1	7.972	942397	20.0
Ethanol, 2-(2-b...	10.566	3.2	ng	221942	2	10.789	1368430	20.0
1-Docosene	21.224	2.5	ng	368868	5	21.512	2944610	20.0
Heneicosane	23.206	3.4	ng	485190	6	23.936	2844750	20.0
Eicosane	23.847	3.5	ng	500112	6	23.936	2844750	20.0
Docosane, 1-iodo-	24.588	4.0	ng	576157	6	23.936	2844750	20.0