LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050224\
Data File : BF137815.D
Acq On : 02 May 2024 15:15
Operator : CG\JU
Sample : P2322-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DEMAREST-MS

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_F\Methods\8270-BF043024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137815.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.216	17	22	28	rVB2	29379	58086	1.23%	0.172%
2	2.446	54	61	67	rBV	290842	379950	8.07%	1.125%
3	3.710	273	276	286	rBV	72061	109618	2.33%	0.325%
4	5.686	606	612	615	rBV	3415282	3453612	73.39%	10.229%
5	6.669	773	779	782	rBV	3089507	3500457	74.38%	10.368%
6	7.057	841	845	848	rBV	1061398	849854	18.06%	2.517%
7	7.616	935	940	943	rBV	2285063	2295120	48.77%	6.798%
8	8.339	1059	1063	1066	rBV	1417924	1149038	24.42%	3.403%
9	8.639	1111	1114	1126	rBV	48216	71442	1.52%	0.212%
10	9.416	1241	1246	1249	rBV	5503833	4705988	100.00%	13.939%
11	10.104	1358	1363	1366	rBV	2387675	2043421	43.42%	6.052%
12	10.186	1372	1377	1390	rBV	1556339	2070742	44.00%	6.133%
13	10.892	1493	1497	1501	rBV	4302509	4223839	89.75%	12.511%
14	11.598	1613	1617	1620	rBV	2366249	1938586	41.19%	5.742%
15	12.104	1699	1703	1720	rBV	800125	792784	16.85%	2.348%
16	12.886	1833	1836	1842	rBV2	116337	115930	2.46%	0.343%
17	13.186	1882	1887	1890	rBV	4723016	4093836	86.99%	12.125%
18	14.121	2039	2046	2058	rBV6	47446	177541	3.77%	0.526%
19	14.245	2063	2067	2071	rBV	894857	749609	15.93%	2.220%
20	15.115	2211	2215	2221	rBV	203106	205671	4.37%	0.609%
21	15.821	2328	2335	2347	rBV	577509	777140	16.51%	2.302%

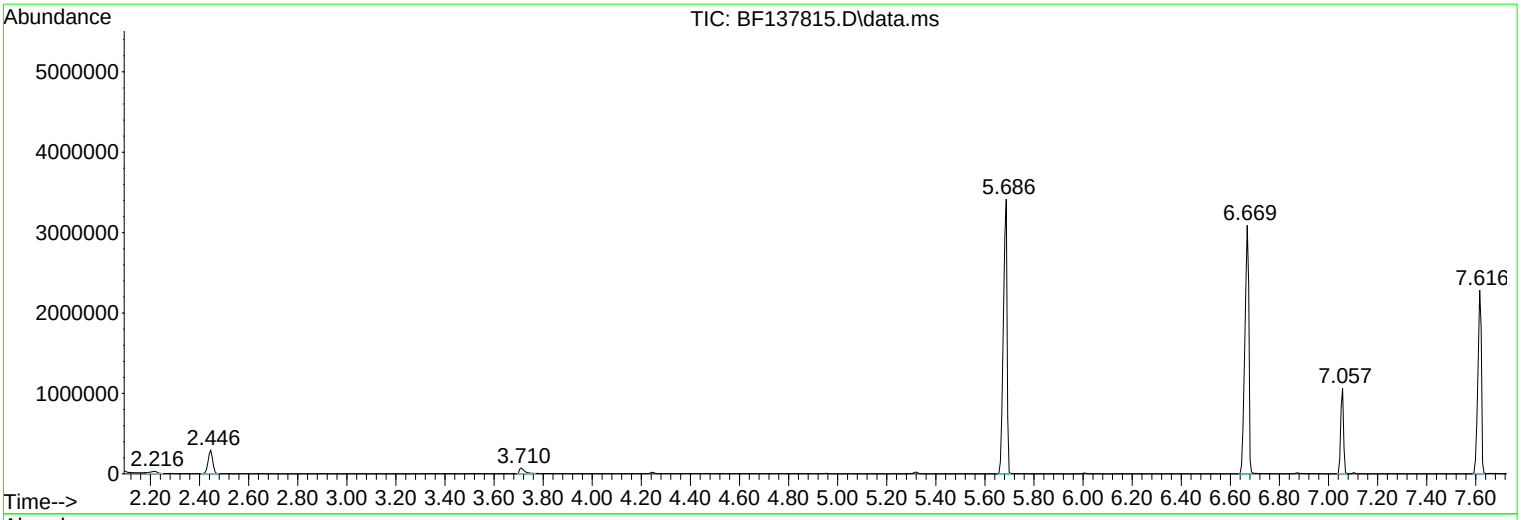
Sum of corrected areas: 33762264

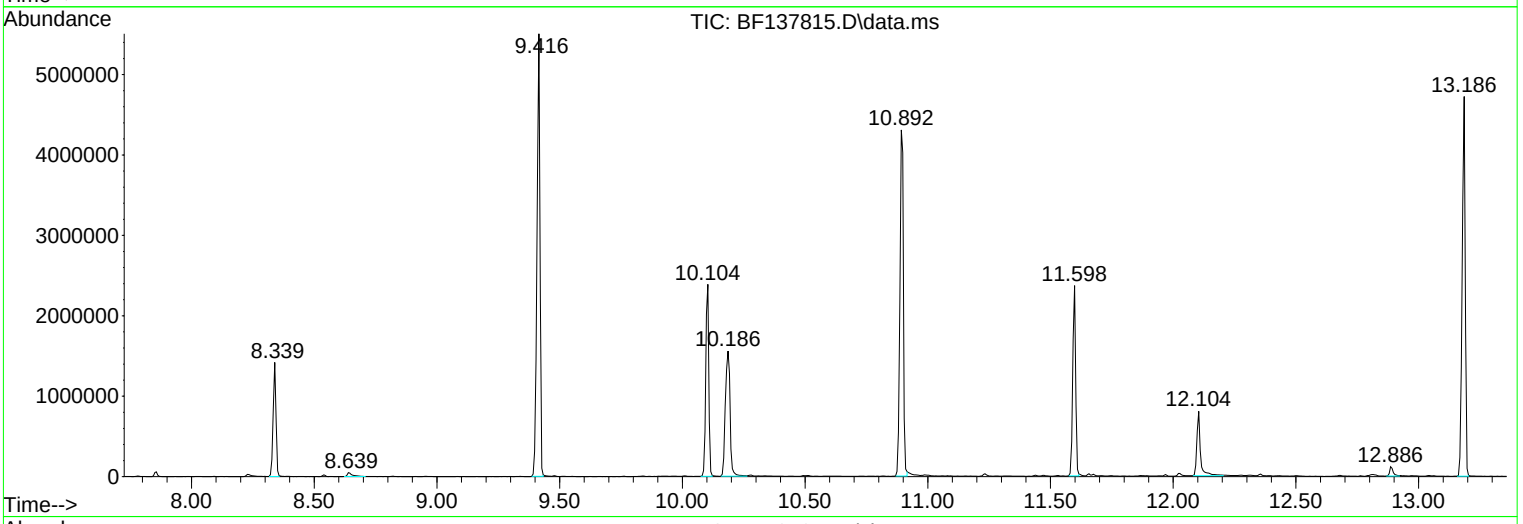
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050224\
Data File : BF137815.D
Acq On : 02 May 2024 15:15
Operator : CG\JU
Sample : P2322-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

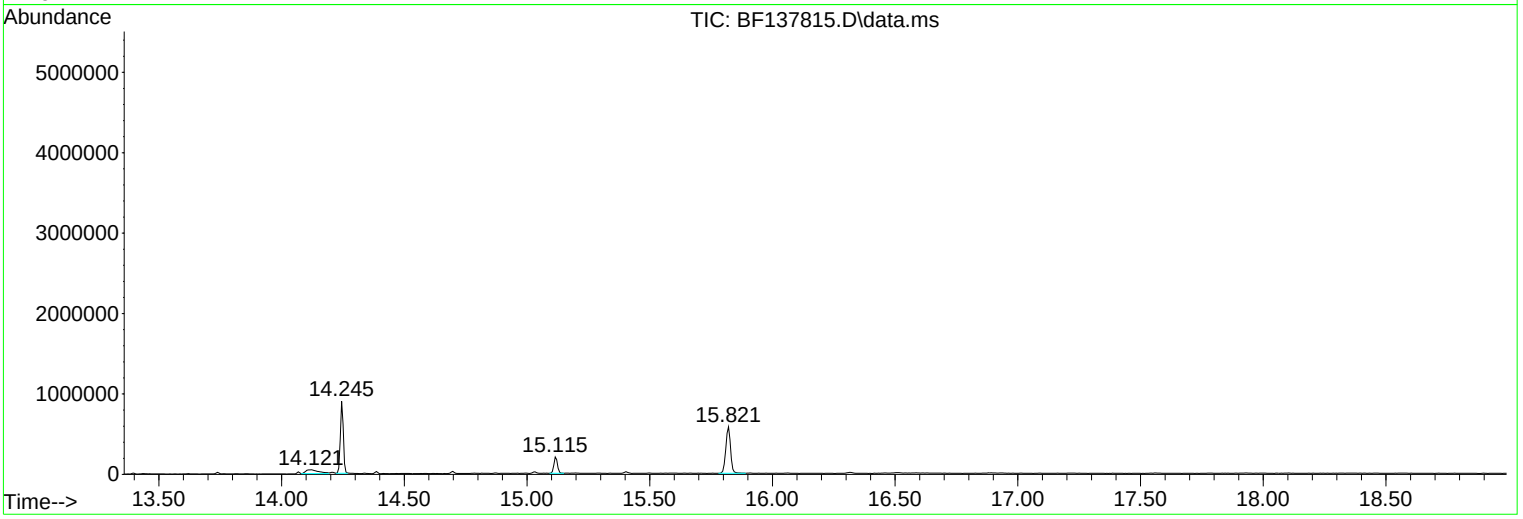
Instrument :
BNA_F
ClientSampleId :
DEMAREST-MS

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043024.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_F\Data\BF050224\
Data File : BF137815.D
Acq On : 02 May 2024 15:15
Operator : CG\JU
Sample : P2322-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DEMAREST-MS

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

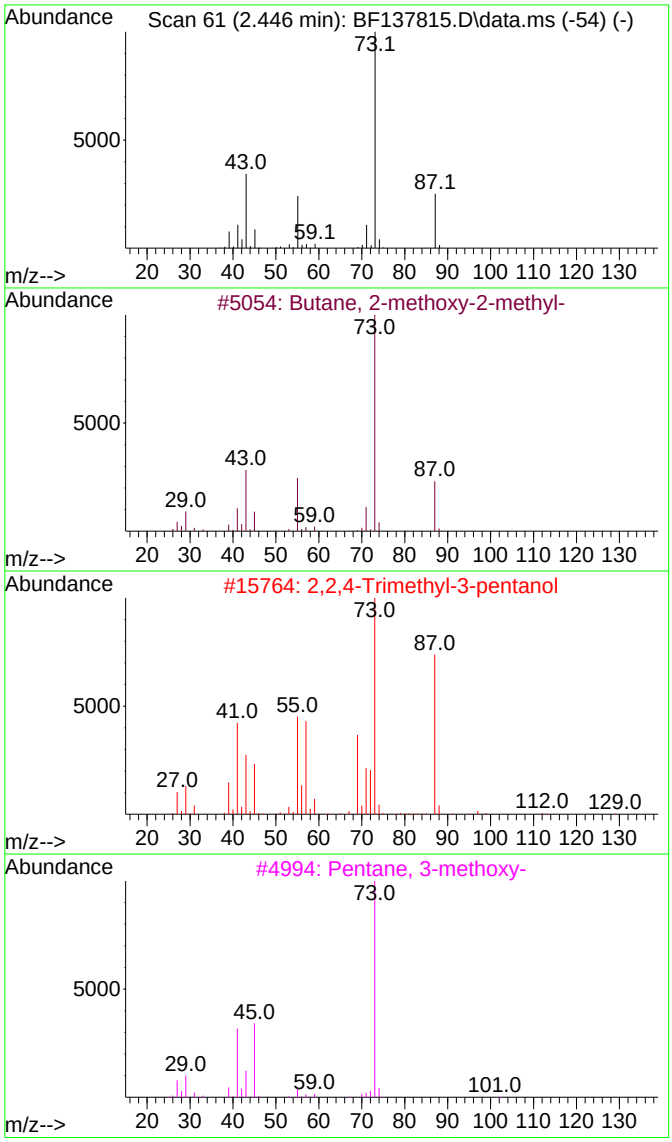
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

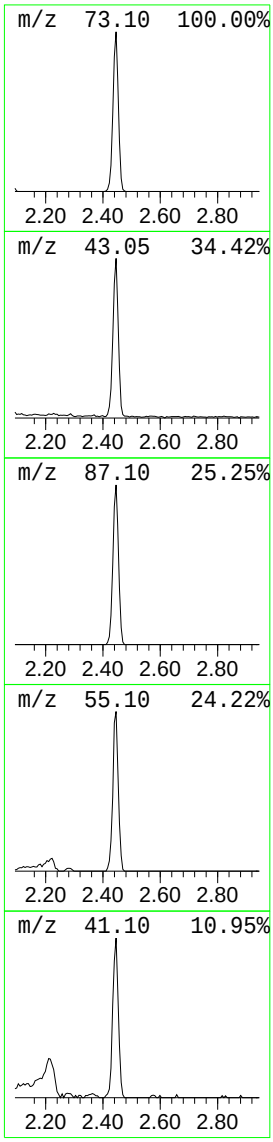
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.446	8.94 ng	379950	1,4-Dichlorobenzene-d4	7.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050224\
Data File : BF137815.D
Acq On : 02 May 2024 15:15
Operator : CG\JU
Sample : P2322-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DEMAREST-MS

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

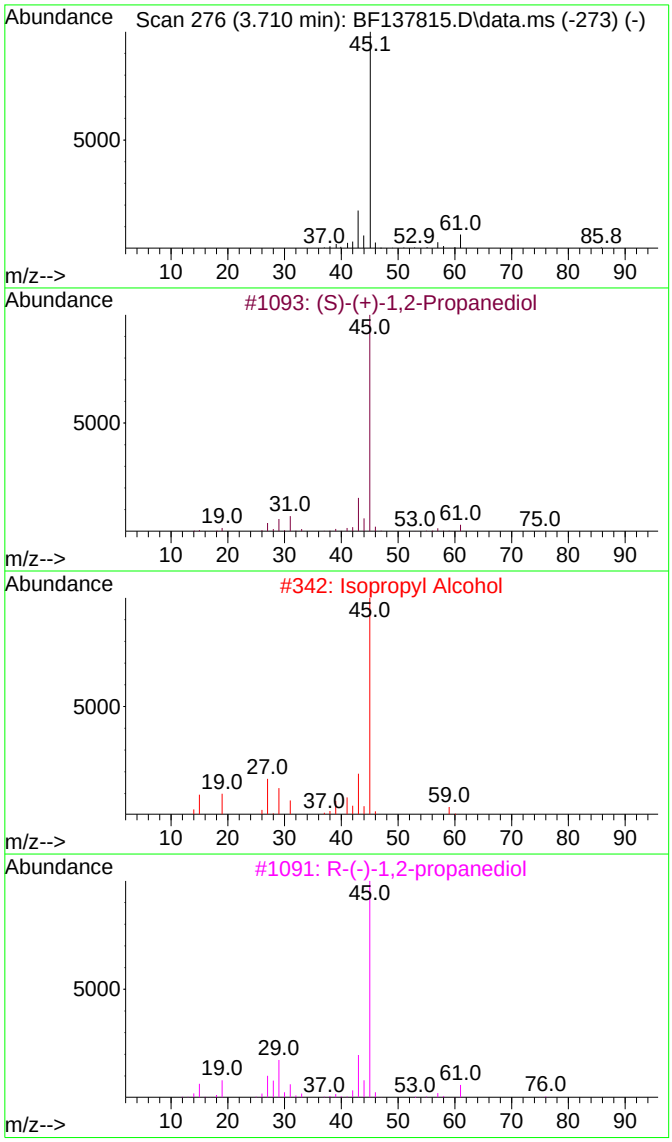
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

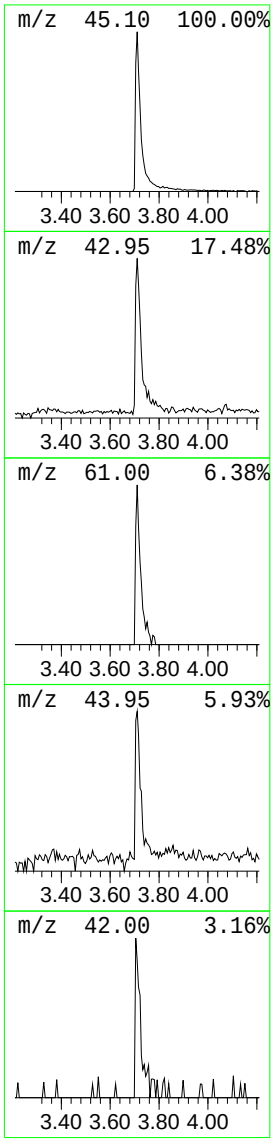
****

Peak Number 2 (S)-(+)-1,2-Propanediol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.710	2.58 ng	109618	1,4-Dichlorobenzene-d4	7.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	56
3	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
4	Propylene Glycol	76	C3H8O2	000057-55-6	9
5	2-Butanol	74	C4H10O	000078-92-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050224\
Data File : BF137815.D
Acq On : 02 May 2024 15:15
Operator : CG\JU
Sample : P2322-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DEMAREST-MS

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

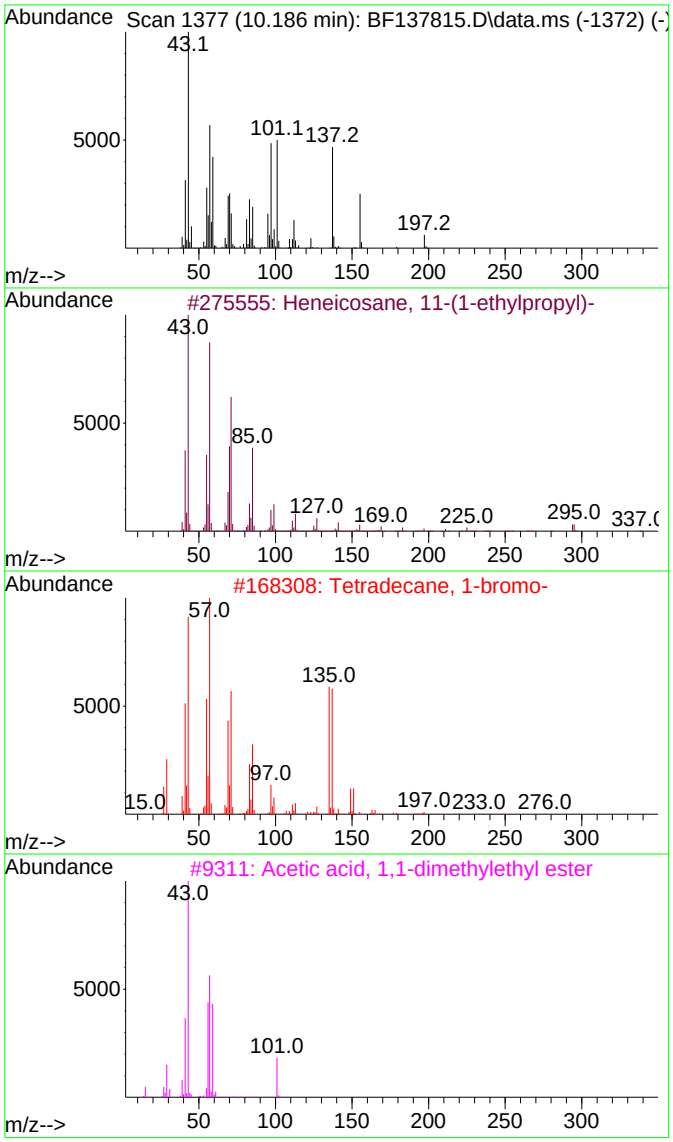
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

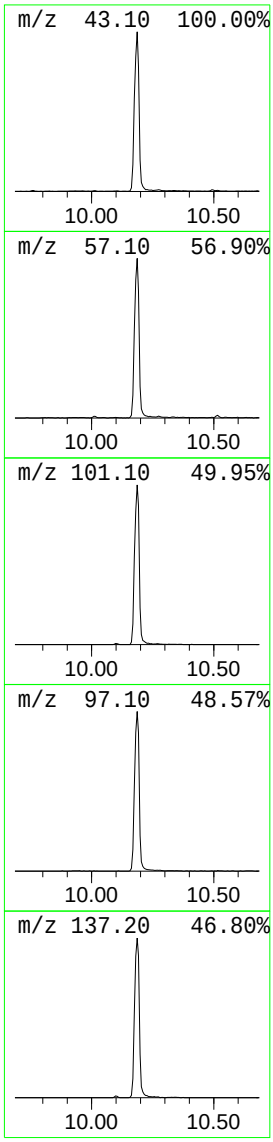
****

Peak Number 3 unknown10.186 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.186	20.27 ng	2070740	Acenaphthene-d10	10.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	10
2	Tetradecane, 1-bromo-	276	C14H29Br	000112-71-0	10
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	10
4	Heptadecane, 1-bromo-	318	C17H35Br	003508-00-7	10
5	Pent-4-enoyl amide, 2-methyl-N-p...	155	C9H17NO	1000420-35-2	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050224\
Data File : BF137815.D
Acq On : 02 May 2024 15:15
Operator : CG\JU
Sample : P2322-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DEMAREST-MS

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

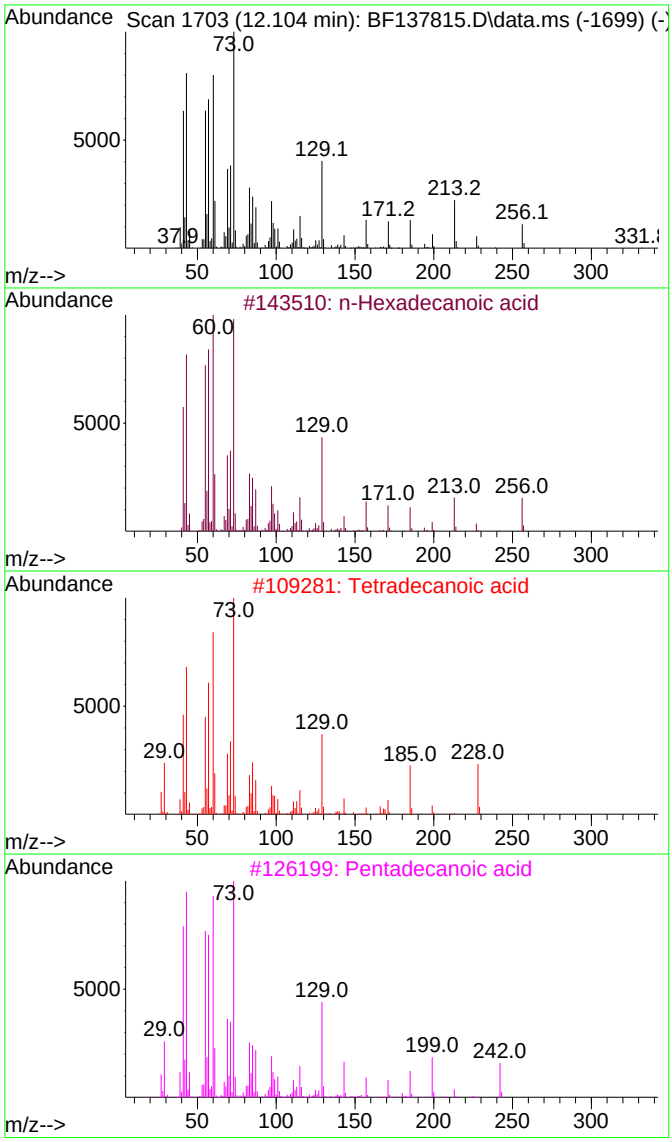
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

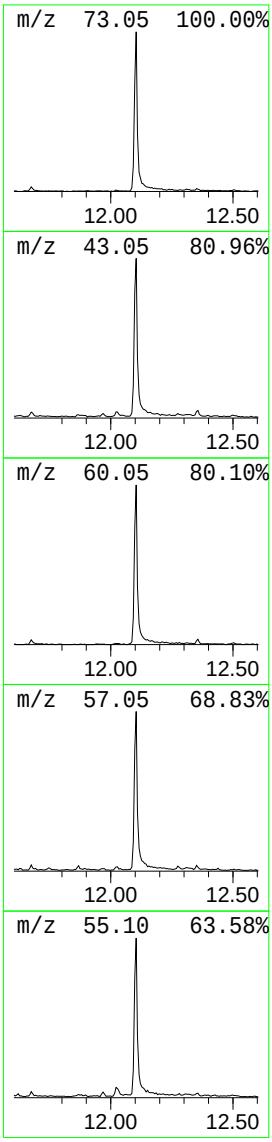
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.104	8.18 ng	792784	Phenanthrene-d10	11.598

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	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tridecanoic acid	214	C13H26O2	000638-53-9	76
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050224\
Data File : BF137815.D
Acq On : 02 May 2024 15:15
Operator : CG\JU
Sample : P2322-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DEMAREST-MS

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

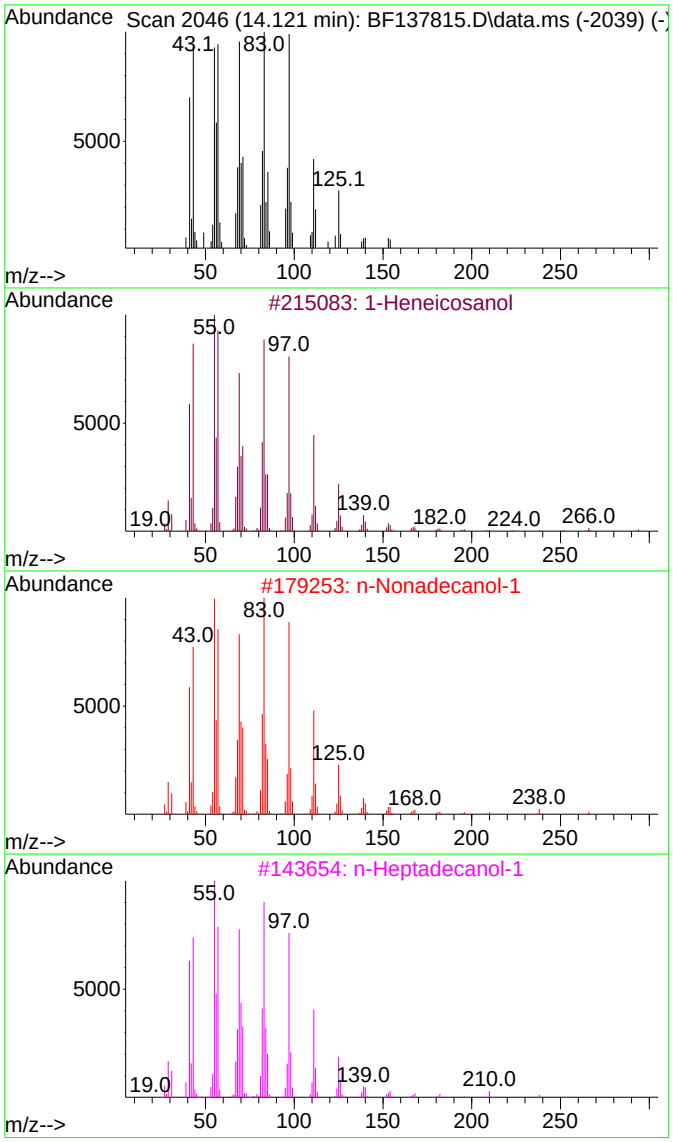
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

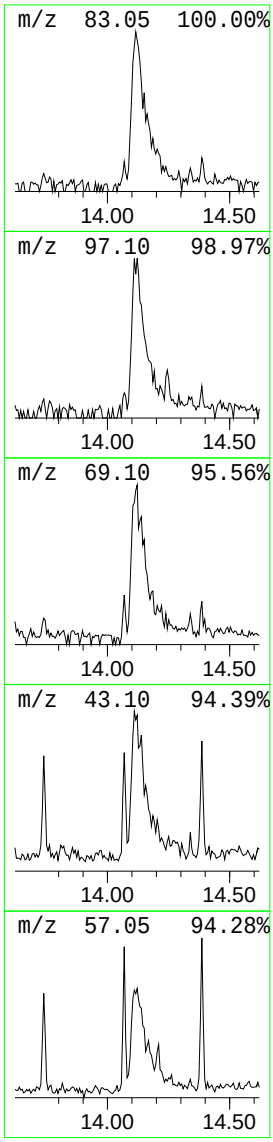
****

Peak Number 5 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.121	4.74 ng	177541	Chrysene-d12	14.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	90
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	90
3	n-Heptadecanol-1	256	C17H36O	001454-85-9	87
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	72
5	Octacosanol	410	C28H58O	000557-61-9	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050224\
Data File : BF137815.D
Acq On : 02 May 2024 15:15
Operator : CG\JU
Sample : P2322-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DEMAREST-MS

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

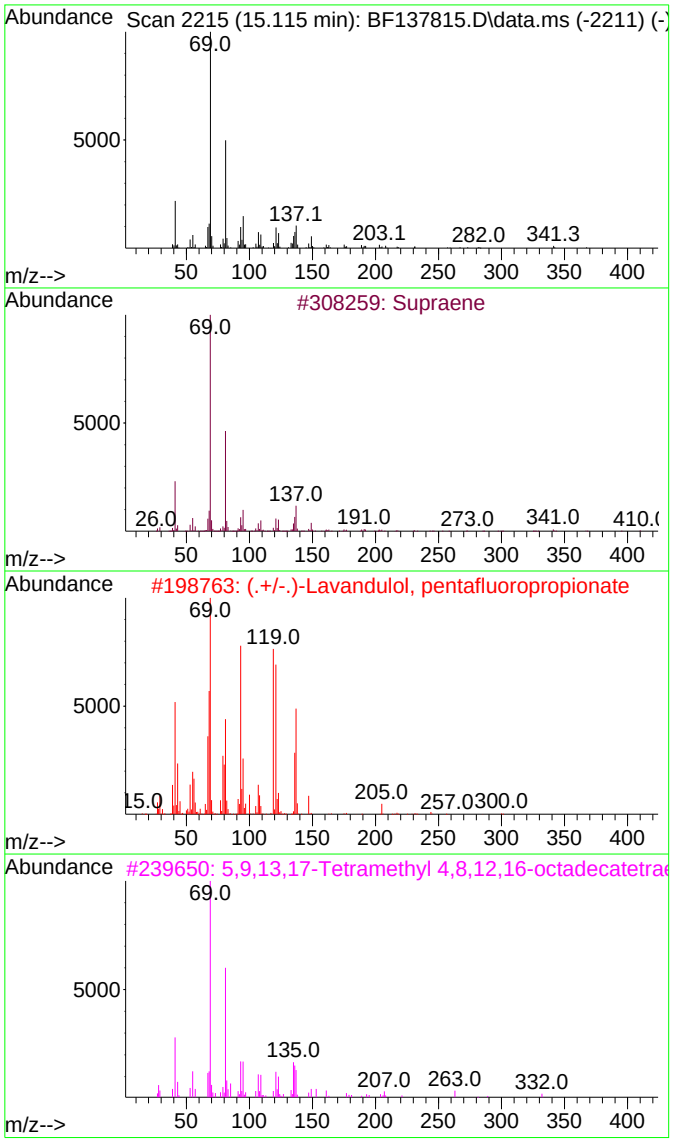
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

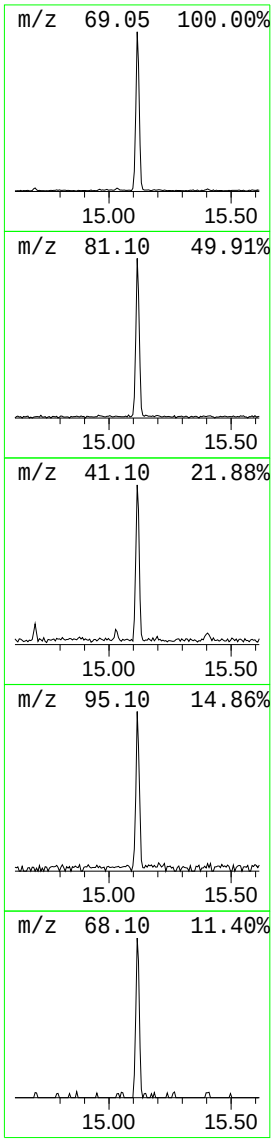
****

Peak Number 6 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.115	5.29 ng	205671	Perylene-d12	15.821

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	(.+/-.)-Lavandulol, pentafluorop...	300	C13H17F5O2	1000352-63-1	72
3	5,9,13,17-Tetramethyl 4,8,12,16-...	332	C22H36O2	1000432-37-9	72
4	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64
5	trans-Farnesol	222	C15H26O	000106-28-5	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050224\
Data File : BF137815.D
Acq On : 02 May 2024 15:15
Operator : CG\JU
Sample : P2322-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DEMAREST-MS

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043024.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
Butane, 2-metho...	2.446	8.9	ng	379950	1	7.057	849854	20.0
(S)-(+)-1,2-Pro...	3.710	2.6	ng	109618	1	7.057	849854	20.0
unknown10.186	10.186	20.3	ng	2070740	3	10.104	2043420	20.0
n-Hexadecanoic ...	12.104	8.2	ng	792784	4	11.598	1938590	20.0
1-Heneicosanol	14.121	4.7	ng	177541	5	14.245	749609	20.0
Supraene	15.115	5.3	ng	205671	6	15.821	777140	20.0