LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030521\
Data File : BM028998.D
Acq On : 05 Mar 2021 16:26
Operator : CG/JU
Sample : M1575-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : IDW-GW805-AQ-030321

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-BM022321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM028998.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.363	60	64	71	rBV	11200	16789	2.85%	0.649%
2	5.245	378	384	392	rVB	83462	116702	19.80%	4.514%
3	5.722	460	465	474	rBV	23890	32461	5.51%	1.256%
4	6.863	654	659	669	rVB	44100	74141	12.58%	2.868%
5	7.675	792	797	803	rVB	38654	55542	9.42%	2.148%
6	8.310	897	905	911	rBV2	8257	14967	2.54%	0.579%
7	8.851	991	997	1007	rBV	111653	174621	29.63%	6.754%
8	9.569	1115	1119	1125	rBV3	4252	6118	1.04%	0.237%
9	9.828	1157	1163	1169	rVB3	5073	7166	1.22%	0.277%
10	9.892	1169	1174	1185	rBV2	12923	21886	3.71%	0.847%
11	10.469	1265	1272	1281	rVB	47237	74303	12.61%	2.874%
12	11.369	1420	1425	1432	rBV	10245	16098	2.73%	0.623%
13	12.957	1689	1695	1703	rBV	253376	358719	60.87%	13.875%
14	13.645	1807	1812	1824	rBV	8756	16521	2.80%	0.639%
15	13.810	1835	1840	1846	rBV	6691	8817	1.50%	0.341%
16	14.345	1926	1931	1938	rVB2	65957	90208	15.31%	3.489%
17	15.845	2180	2186	2192	rBV	226848	304892	51.73%	11.793%
18	17.092	2392	2398	2404	rBV	79178	103707	17.60%	4.011%
19	17.992	2546	2551	2562	rBV	39719	55365	9.39%	2.141%
20	18.733	2673	2677	2682	rBV	14878	17147	2.91%	0.663%
21	19.274	2764	2769	2777	rBV	23308	32140	5.45%	1.243%
22	19.721	2839	2845	2851	rBV	507761	589342	100.00%	22.795%
23	20.227	2926	2931	2944	rBV	30853	49414	8.38%	1.911%
24	20.980	3055	3059	3066	rBV	50871	65698	11.15%	2.541%
25	21.268	3103	3108	3115	rBV	114614	135819	23.05%	5.253%
26	23.427	3470	3475	3484	rVB2	81897	146825	24.91%	5.679%

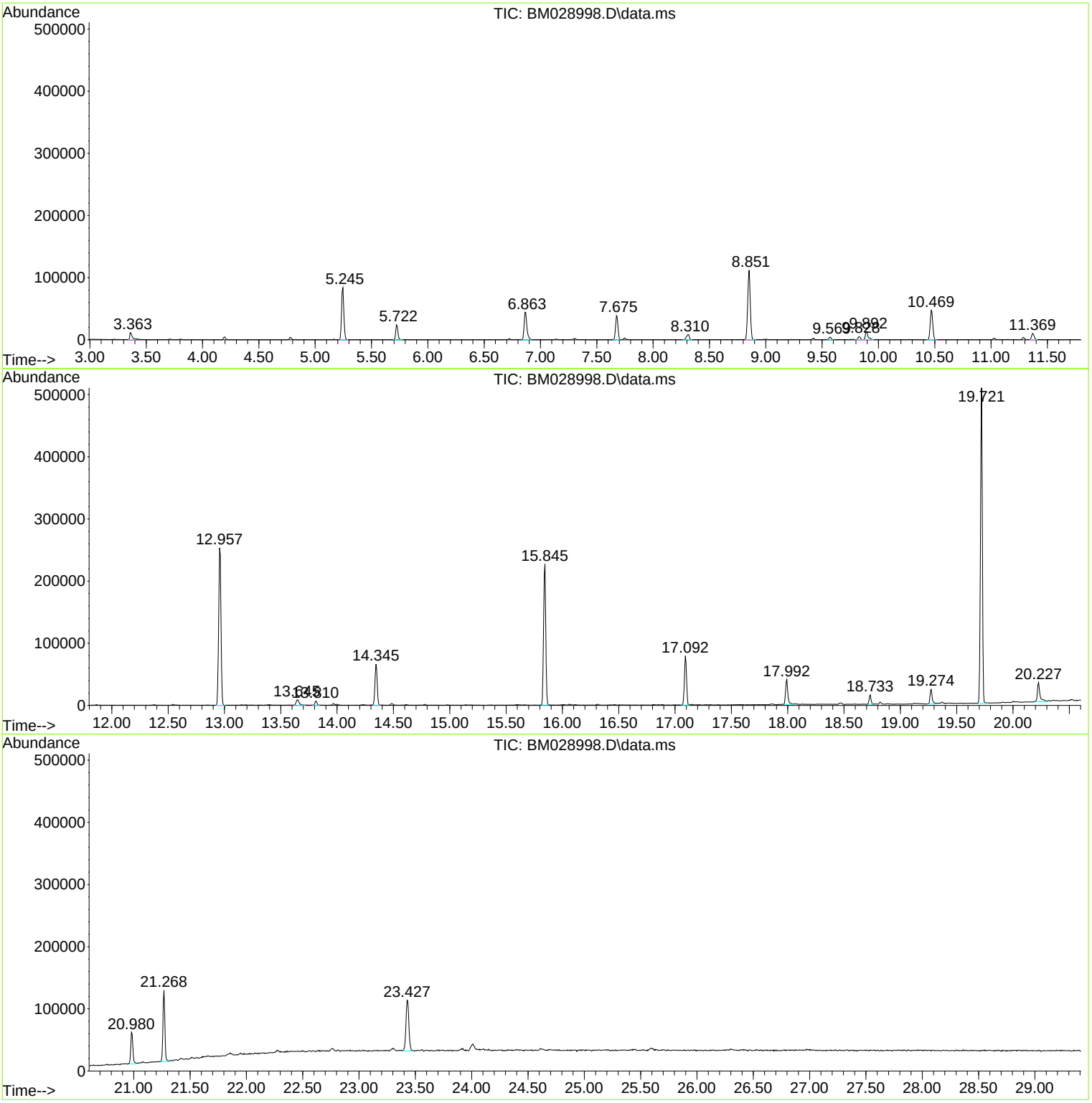
Sum of corrected areas: 2585408

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030521\
Data File : BM028998.D
Acq On : 05 Mar 2021 16:26
Operator : CG/JU
Sample : M1575-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
IDW-GW805-AQ-030321

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030521\
Data File : BM028998.D
Acq On : 05 Mar 2021 16:26
Operator : CG/JU
Sample : M1575-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
IDW-GW805-AQ-030321

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

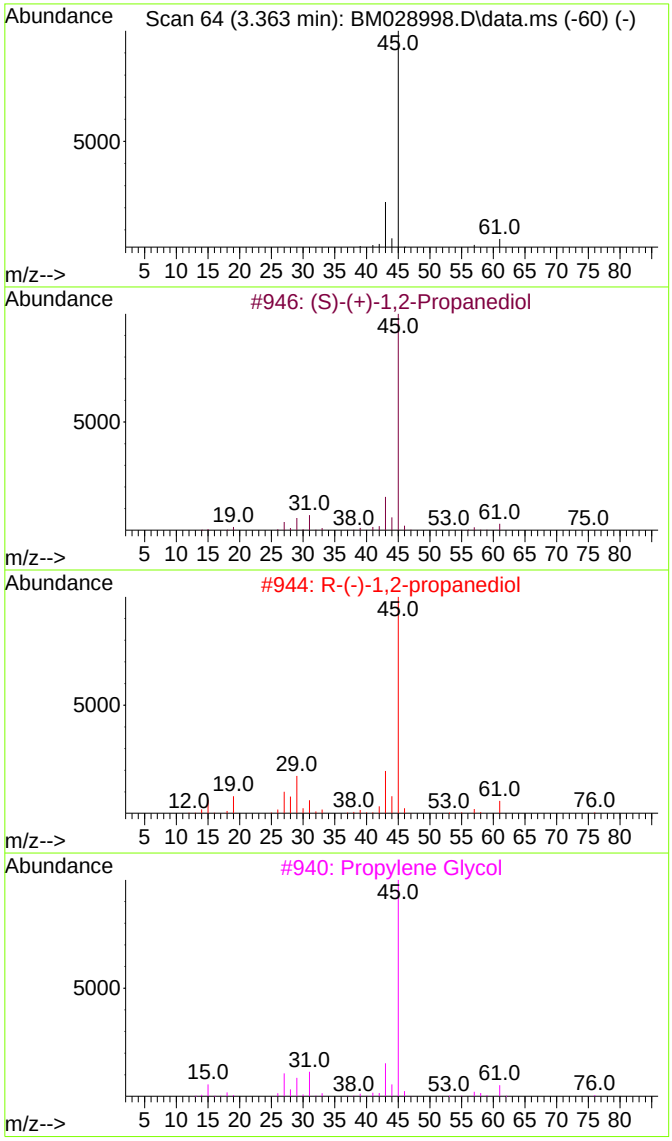
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

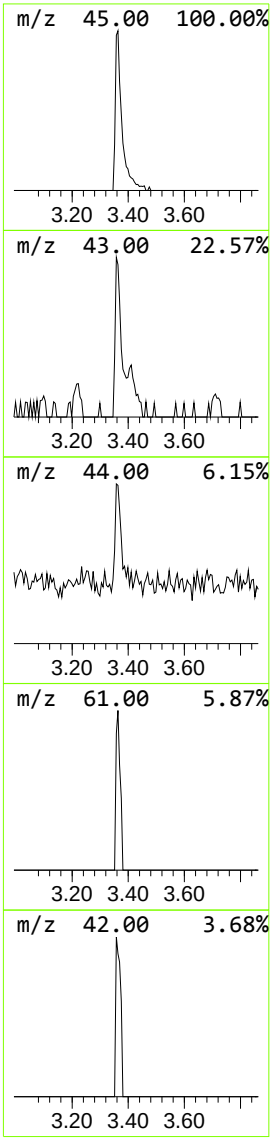
****

Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.363	6.05 ng	16789	1,4-Dichlorobenzene-d4	7.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
3	Propylene Glycol	76	C3H8O2	000057-55-6	9
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5	Formamide	45	CH3NO	000075-12-7	5





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030521\
Data File : BM028998.D
Acq On : 05 Mar 2021 16:26
Operator : CG/JU
Sample : M1575-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
IDW-GW805-AQ-030321

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

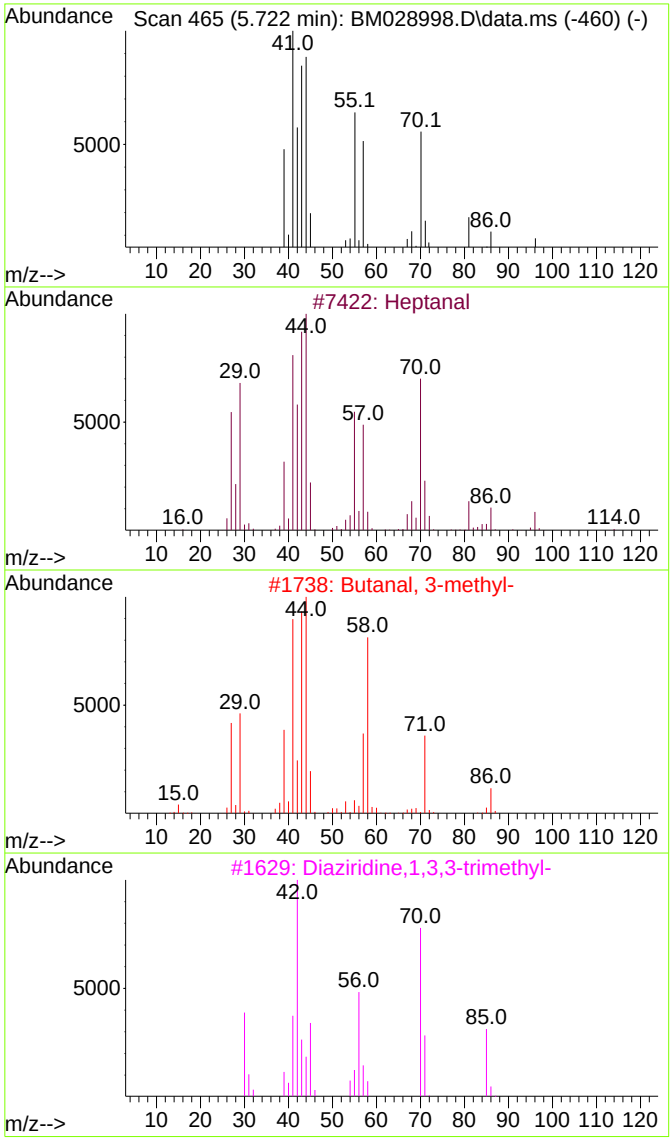
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

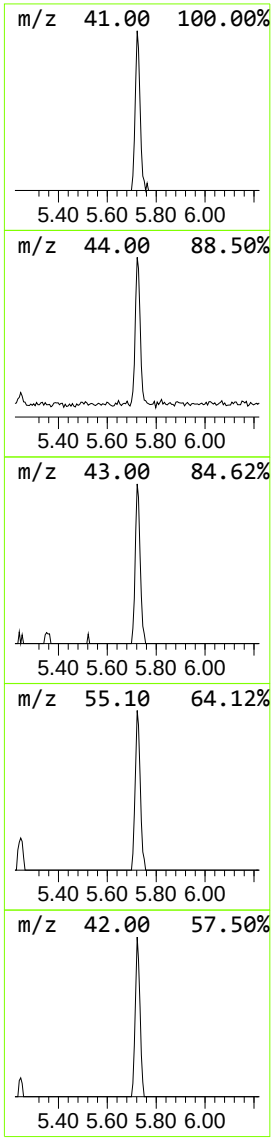
****

Peak Number 2 Heptanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.722	11.69 ng	32461	1,4-Dichlorobenzene-d4	7.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanal	114	C7H14O	000111-71-7	72
2	Butanal, 3-methyl-	86	C5H10O	000590-86-3	58
3	Diaziridine,1,3,3-trimethyl-	86	C4H10N2	040711-15-7	35
4	2-Pentene, (Z)-	70	C5H10	000627-20-3	25
5	2-Pentene, (E)-	70	C5H10	000646-04-8	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030521\
Data File : BM028998.D
Acq On : 05 Mar 2021 16:26
Operator : CG/JU
Sample : M1575-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : IDW-GW805-AQ-030321

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

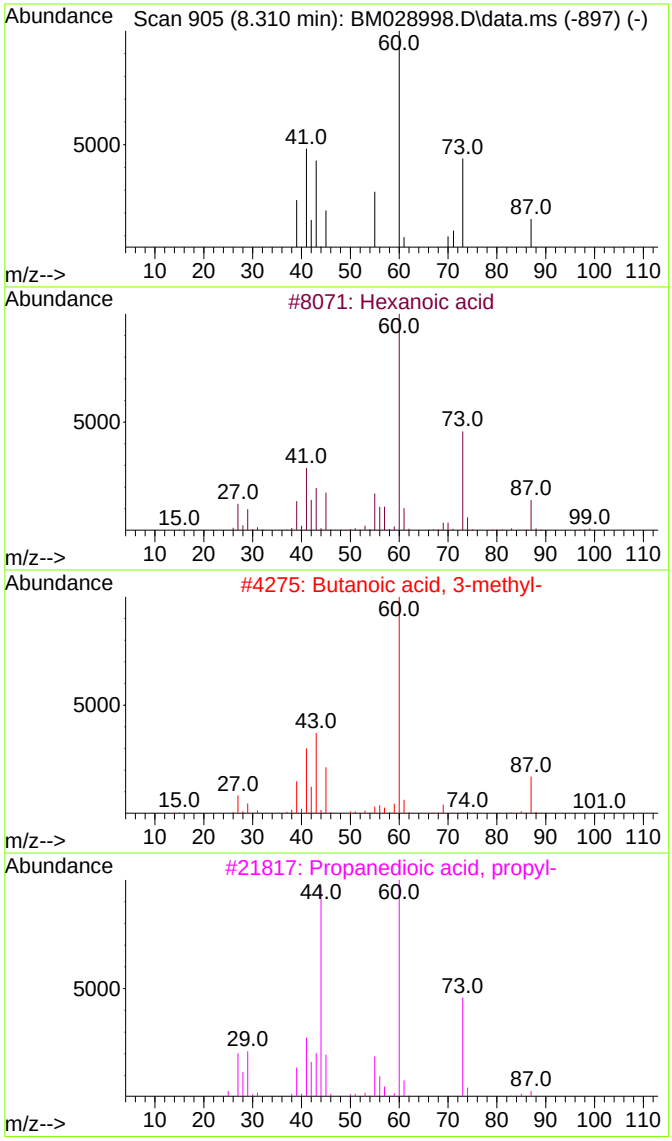
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

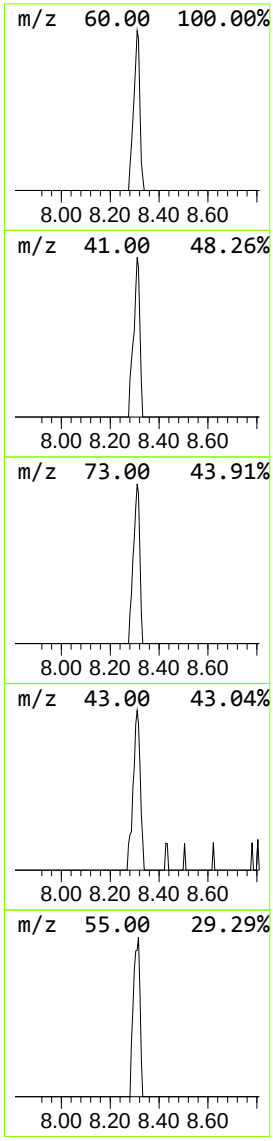
****

Peak Number 3 Hexanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.310	5.39 ng	14967	1,4-Dichlorobenzene-d4	7.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid	116	C6H12O2	000142-62-1	78
2	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	50
3	Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	39
4	Formic acid hydrazide	60	CH4N2O	000624-84-0	28
5	3-Methyl-hexanoic acid	130	C7H14O2	1000365-65-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030521\
Data File : BM028998.D
Acq On : 05 Mar 2021 16:26
Operator : CG/JU
Sample : M1575-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : IDW-GW805-AQ-030321

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

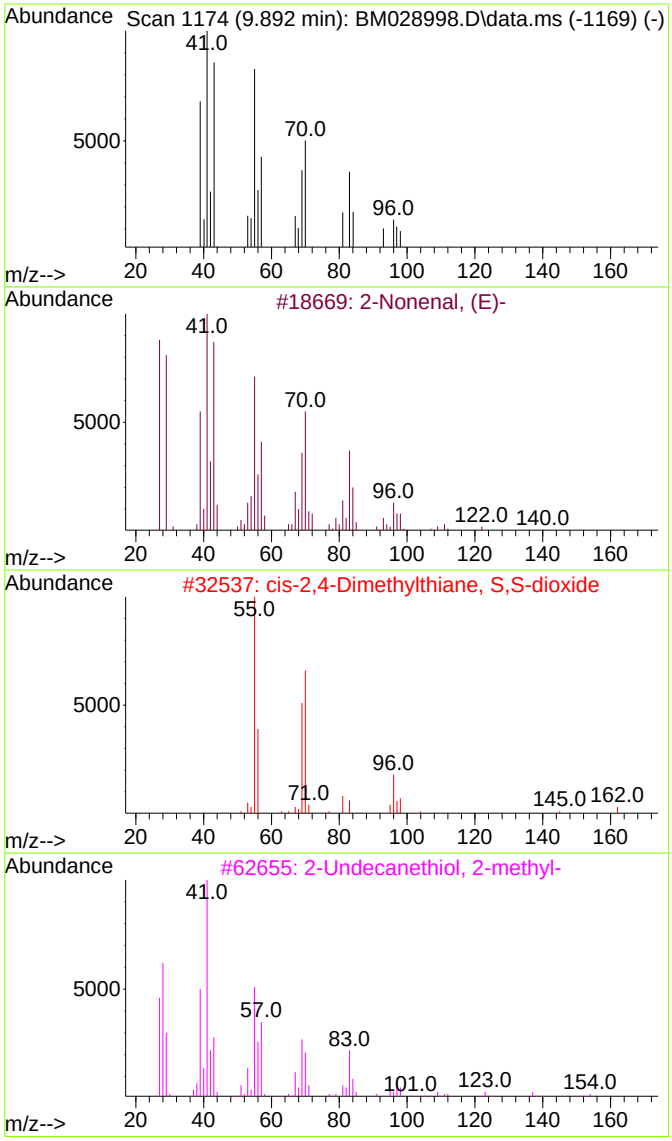
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

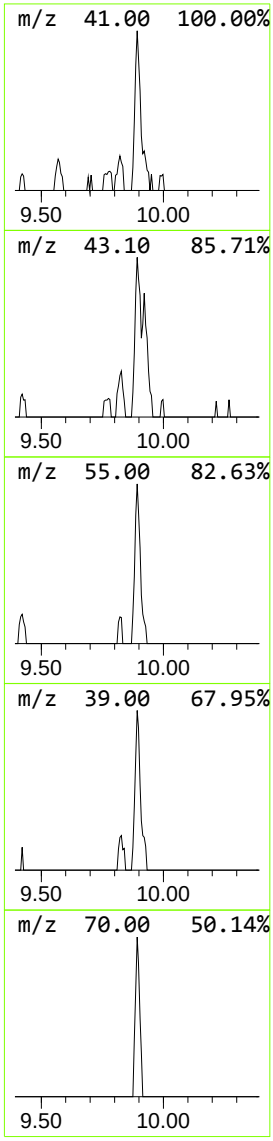
****

Peak Number 4 2-Nonenal, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.892	5.89 ng	21886	Naphthalene-d8	10.469

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Nonenal, (E)-	140	C9H16O	018829-56-6	86
2	cis-2,4-Dimethylthiane, S,S-dioxide	162	C7H14O2S	1000215-67-5	59
3	2-Undecanethiol, 2-methyl-	202	C12H26S	010059-13-9	59
4	Methacrolein	70	C4H6O	000078-85-3	43
5	1-Heptyn-3-ol	112	C7H12O	007383-19-9	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030521\
Data File : BM028998.D
Acq On : 05 Mar 2021 16:26
Operator : CG/JU
Sample : M1575-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
IDW-GW805-AQ-030321

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

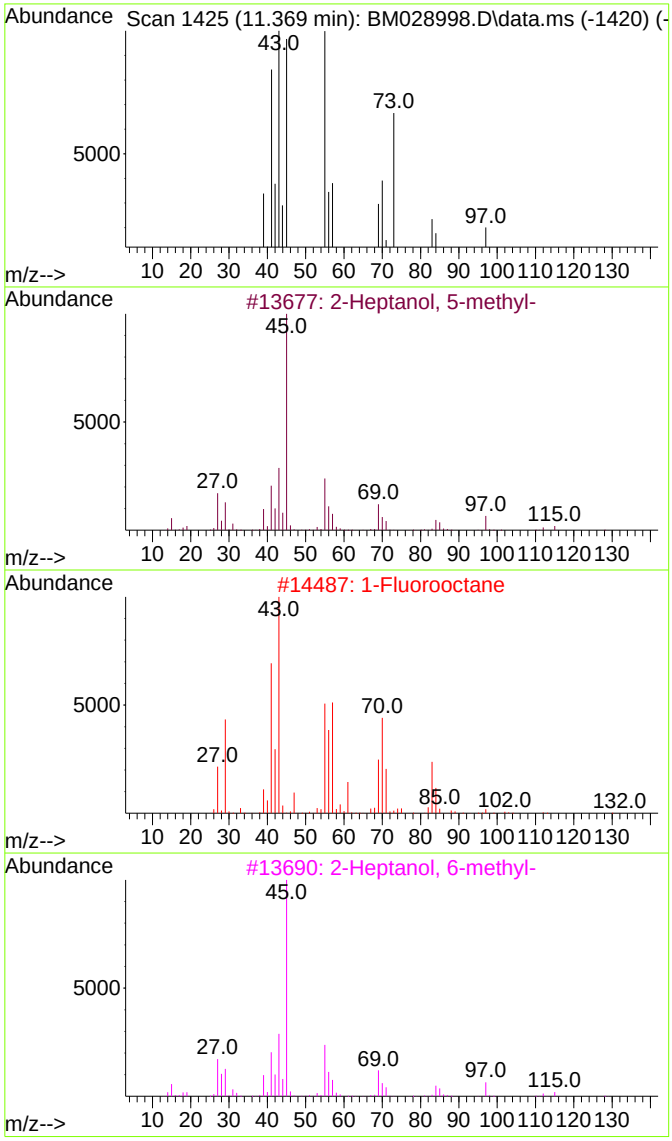
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

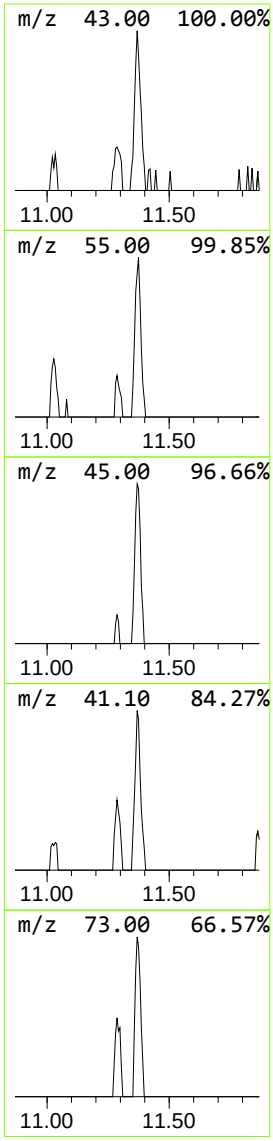
****

Peak Number 5 unknown11.36 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.369	4.33 ng	16098	Naphthalene-d8	10.469

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanol, 5-methyl-	130	C8H18O	054630-50-1	25
2	1-Fluorooctane	132	C8H17F	000463-11-6	25
3	2-Heptanol, 6-methyl-	130	C8H18O	004730-22-7	25
4	1-Heptyn-3-ol	112	C7H12O	007383-19-9	23
5	2-Octanol, (S)-	130	C8H18O	006169-06-8	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030521\
Data File : BM028998.D
Acq On : 05 Mar 2021 16:26
Operator : CG/JU
Sample : M1575-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
IDW-GW805-AQ-030321

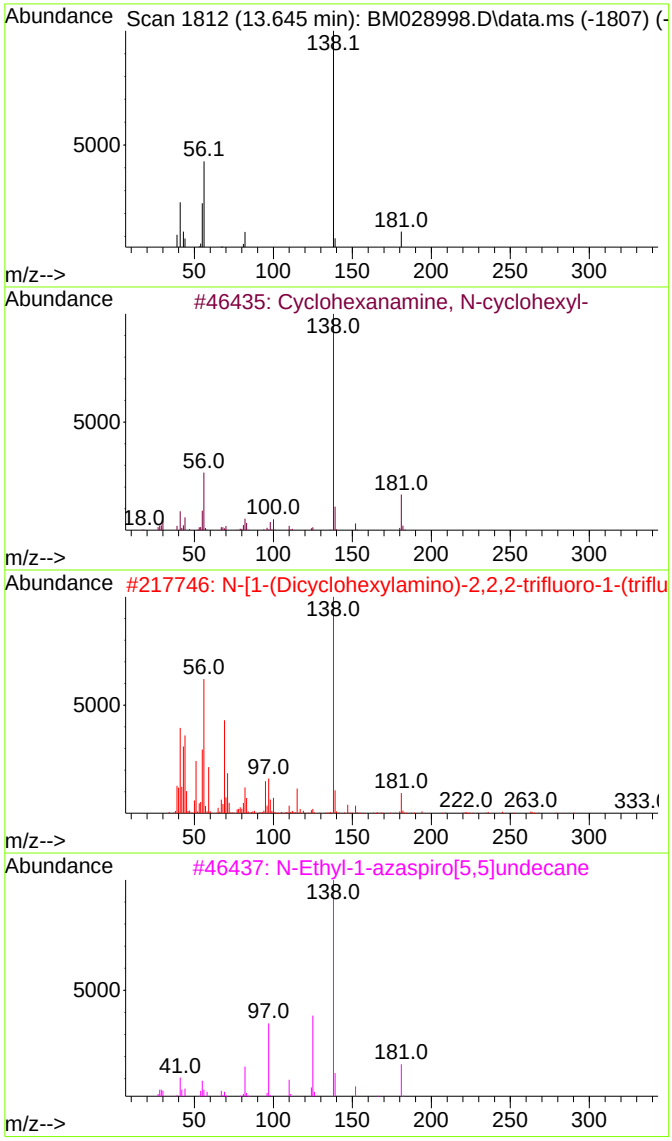
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

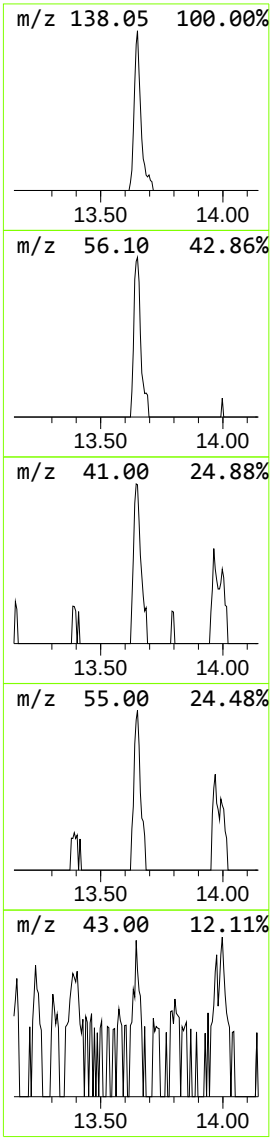
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Cyclohexanamine, N-cyclohexyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.645	3.66 ng	16521	Acenaphthene-d10	14.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanamine, N-cyclohexyl-	181	C12H23N	000101-83-7	72
2	N-[1-(Dicyclohexylamino)-2,2,2-t...	416	C19H30F6N2O	1000225-27-8	39
3	N-Ethyl-1-azaspiro[5,5]undecane	181	C12H23N	1000101-78-6	38
4	4,6-Dimethyl-2-pyrimidinylhydrazine	138	C6H10N4	023906-13-0	9
5	3-Pyridinecarboxamide, 1,6-dihyd...	138	C6H6N2O2	003670-59-5	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030521\
Data File : BM028998.D
Acq On : 05 Mar 2021 16:26
Operator : CG/JU
Sample : M1575-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
IDW-GW805-AQ-030321

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

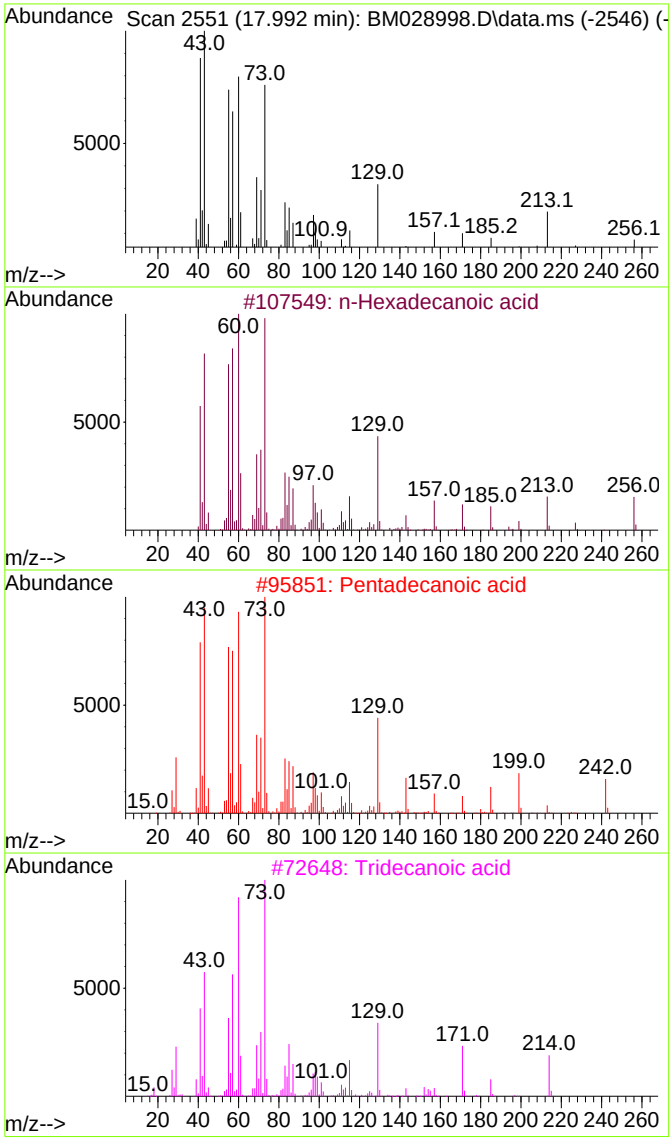
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

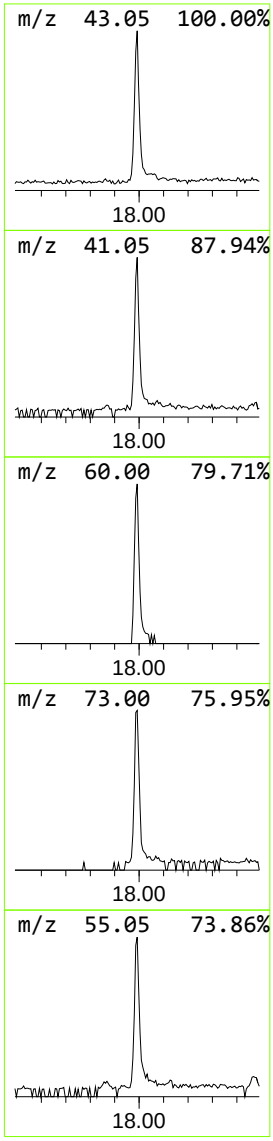
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.992	10.68 ng	55365	Phenanthrene-d10	17.092

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Tridecanoic acid	214	C13H26O2	000638-53-9	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5	Undecanoic acid	186	C11H22O2	000112-37-8	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030521\
Data File : BM028998.D
Acq On : 05 Mar 2021 16:26
Operator : CG/JU
Sample : M1575-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
IDW-GW805-AQ-030321

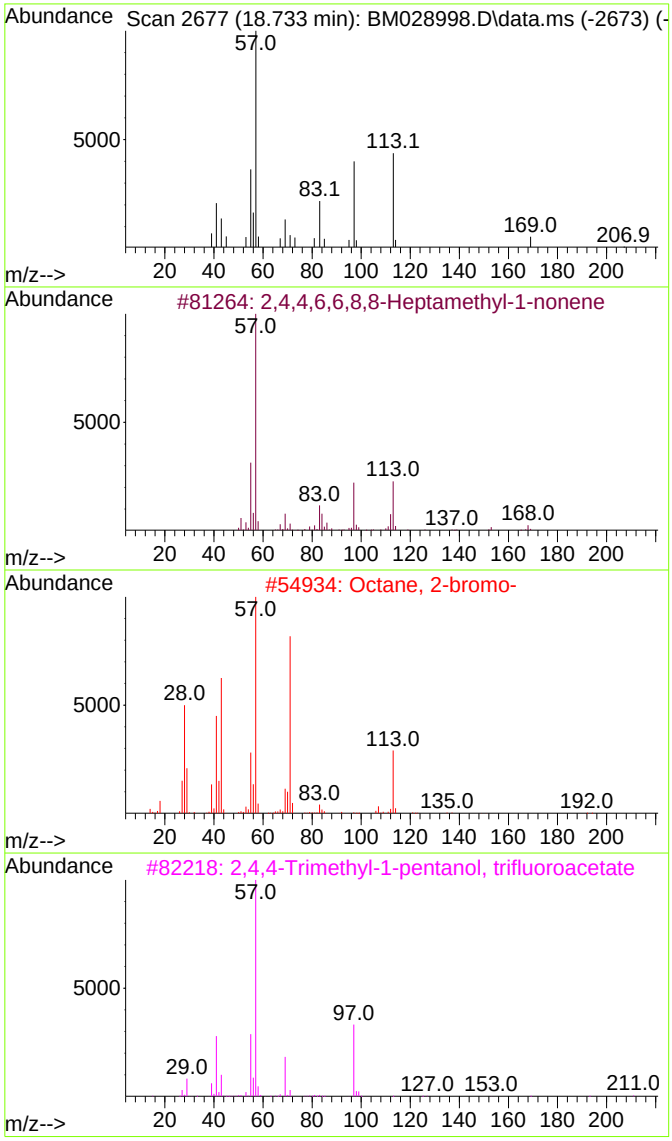
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

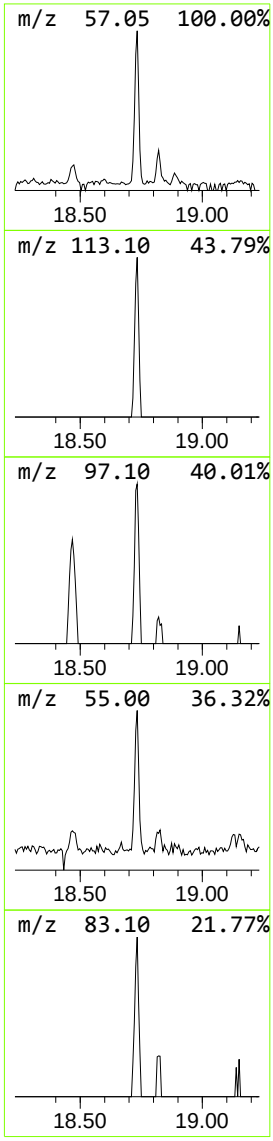
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.733	3.31 ng	17147	Phenanthrene-d10	17.092

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	78
2	Octane, 2-bromo-	192	C8H17Br	000557-35-7	35
3	2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2	1000365-19-5	27
4	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	27
5	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030521\
Data File : BM028998.D
Acq On : 05 Mar 2021 16:26
Operator : CG/JU
Sample : M1575-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : IDW-GW805-AQ-030321

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

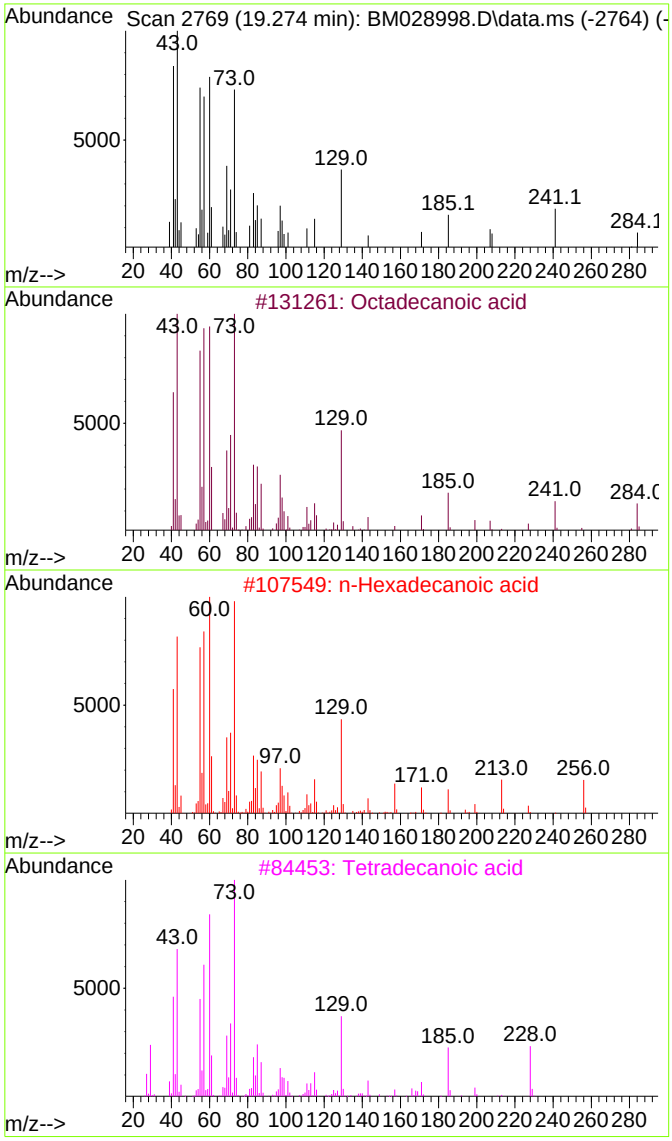
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

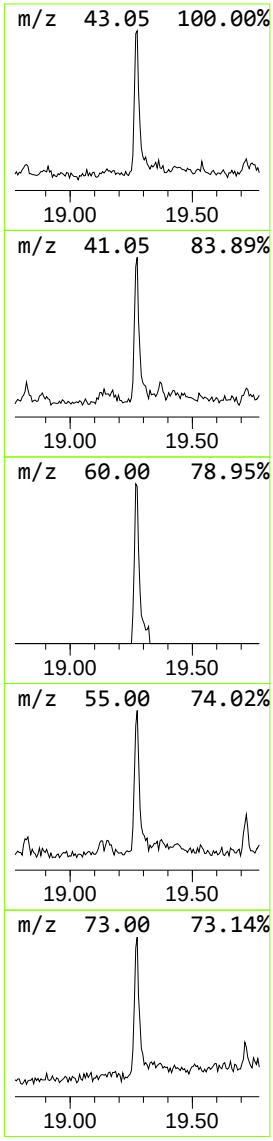
****

Peak Number 9 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.274	4.73 ng	32140	Chrysene-d12	21.268

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	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5	Tridecanoic acid	214	C13H26O2	000638-53-9	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030521\
Data File : BM028998.D
Acq On : 05 Mar 2021 16:26
Operator : CG/JU
Sample : M1575-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : IDW-GW805-AQ-030321

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

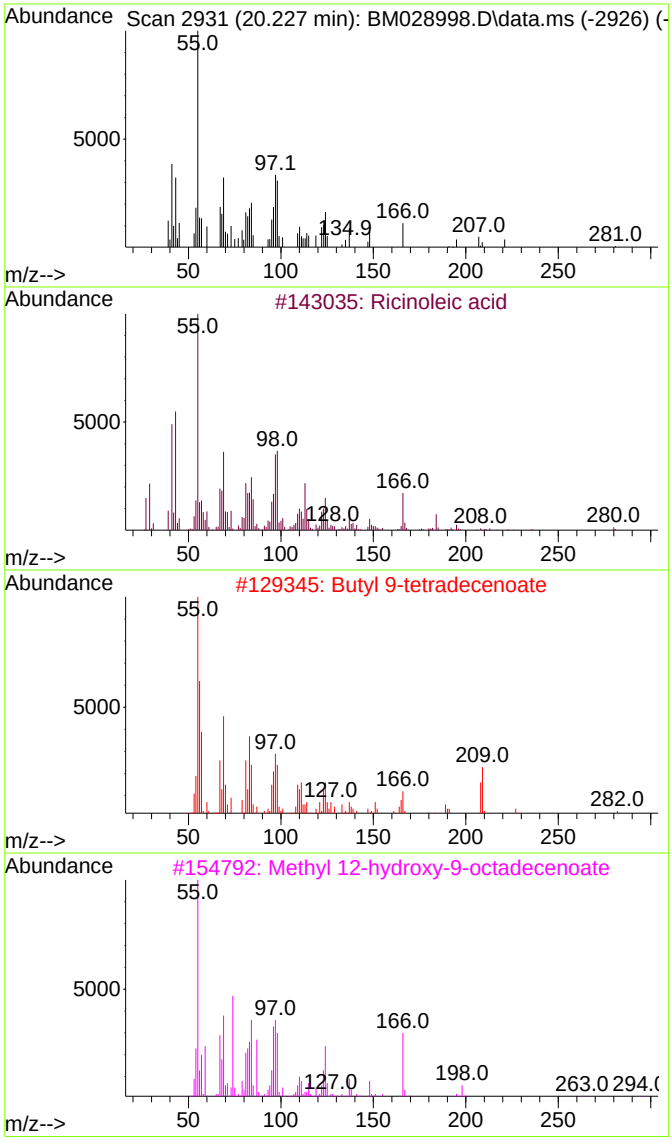
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

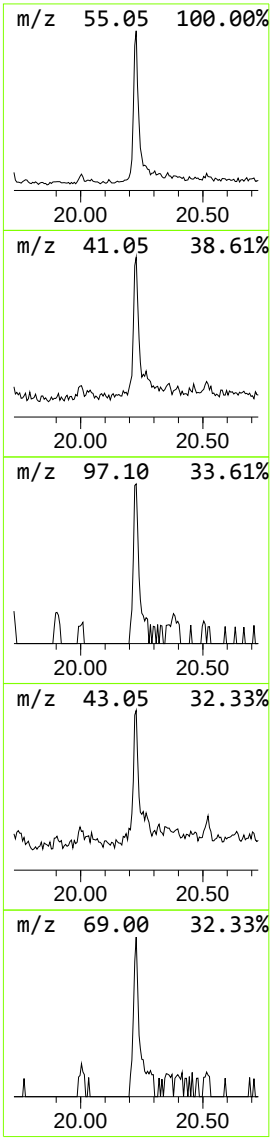
****

Peak Number 10 Ricinoleic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.227	7.28 ng	49414	Chrysene-d12	21.268

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ricinoleic acid	298	C18H34O3	000141-22-0	86
2	Butyl 9-tetradecenoate	282	C18H34O2	1000336-51-4	64
3	Methyl 12-hydroxy-9-octadecenoate	312	C19H36O3	1000336-28-8	58
4	9-Octadecenoic acid, 12-hydroxy-...	312	C19H36O3	000141-24-2	52
5	Chloromethyl 5-chloroundecanoate	268	C12H22Cl2O2	080418-91-3	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030521\
Data File : BM028998.D
Acq On : 05 Mar 2021 16:26
Operator : CG/JU
Sample : M1575-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
IDW-GW805-AQ-030321

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

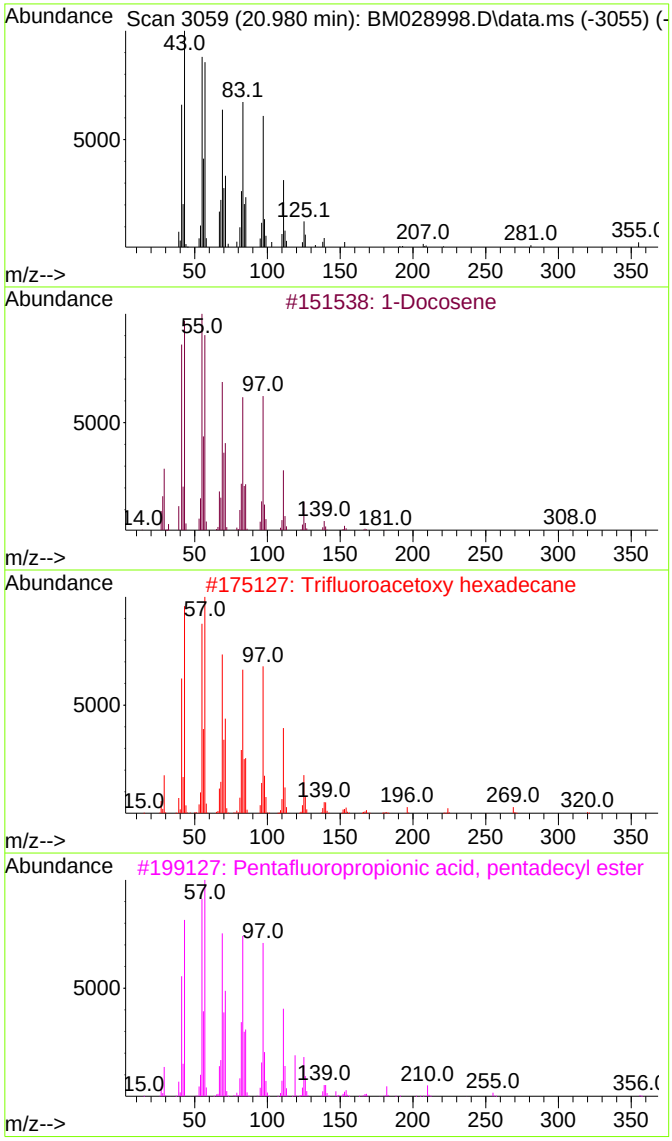
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

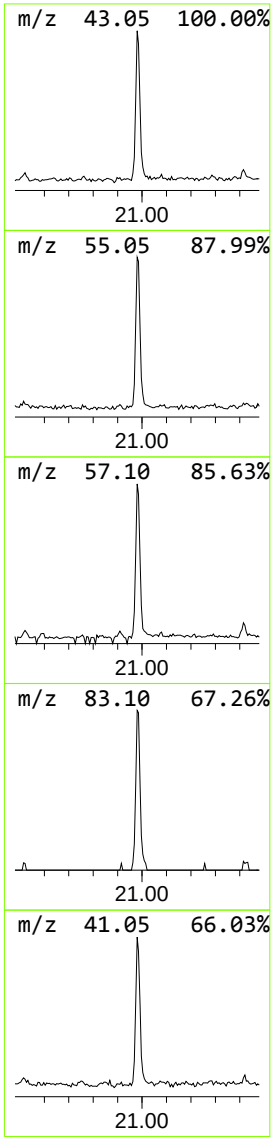
****

Peak Number 11 1-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.980	9.67 ng	65698	Chrysene-d12	21.268

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	95
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
4	1-Hexadecanol	242	C16H34O	036653-82-4	91
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030521\
Data File : BM028998.D
Acq On : 05 Mar 2021 16:26
Operator : CG/JU
Sample : M1575-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : IDW-GW805-AQ-030321

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(S)-(+)-1,2-Pro...	3.363	6.0	ng	16789	1	7.675	55542	20.0
Heptanal	5.722	11.7	ng	32461	1	7.675	55542	20.0
Hexanoic acid	8.310	5.4	ng	14967	1	7.675	55542	20.0
2-Nonenal, (E)-	9.892	5.9	ng	21886	2	10.469	74303	20.0
unknown11.36	11.369	4.3	ng	16098	2	10.469	74303	20.0
Cyclohexanamine...	13.645	3.7	ng	16521	3	14.345	90208	20.0
n-Hexadecanoic ...	17.992	10.7	ng	55365	4	17.092	103707	20.0
2,4,4,6,6,8,8-H...	18.733	3.3	ng	17147	4	17.092	103707	20.0
Octadecanoic acid	19.274	4.7	ng	32140	5	21.268	135819	20.0
Ricinoleic acid	20.227	7.3	ng	49414	5	21.268	135819	20.0
1-Docosene	20.980	9.7	ng	65698	5	21.268	135819	20.0