LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM071025\
Data File : BM050390.D
Acq On : 10 Jul 2025 15:17
Operator : RC/JU
Sample : Q2529-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-79

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-BM070925.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM050390.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.040	4	9	27	rVB	1771767	2453880	4.53%	1.136%
2	4.975	330	338	344	rBV	717847	1049421	1.94%	0.486%
3	5.440	408	417	427	rBV	8482264	12400742	22.91%	5.743%
4	7.022	677	686	703	rBV	8435992	13332626	24.63%	6.175%
5	7.863	822	829	836	rBV	1780215	2809234	5.19%	1.301%
6	9.016	1015	1025	1037	rBV	5197592	8373943	15.47%	3.878%
7	10.657	1296	1304	1312	rBV	2199531	3662763	6.77%	1.696%
8	13.116	1715	1722	1729	rBV	13016509	19458660	35.95%	9.012%
9	14.492	1949	1956	1962	rBV	3261733	4848226	8.96%	2.245%
10	15.727	2144	2166	2170	rBV2	680885	3191247	5.90%	1.478%
11	15.845	2181	2186	2200	rVB	1131155	1878519	3.47%	0.870%
12	15.968	2201	2207	2216	rBV	11694688	16676270	30.81%	7.723%
13	16.162	2219	2240	2284	rBV	12757873	54130850	100.00%	25.069%
14	17.221	2415	2420	2426	rBV2	4217992	5936069	10.97%	2.749%
15	18.127	2567	2574	2593	rBV	5792133	9342103	17.26%	4.326%
16	19.274	2761	2769	2781	rBV7	223799	721942	1.33%	0.334%
17	19.398	2785	2790	2811	rVV	2142503	3574094	6.60%	1.655%
18	19.839	2860	2865	2874	rVB	28439754	35710318	65.97%	16.538%
19	21.133	3080	3085	3098	rBV	1442860	2264765	4.18%	1.049%
20	21.450	3133	3139	3154	rBV	4915443	7262446	13.42%	3.363%
21	24.491	3647	3656	3668	rVB	2777810	6849487	12.65%	3.172%

Sum of corrected areas: 215927605

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM071025\
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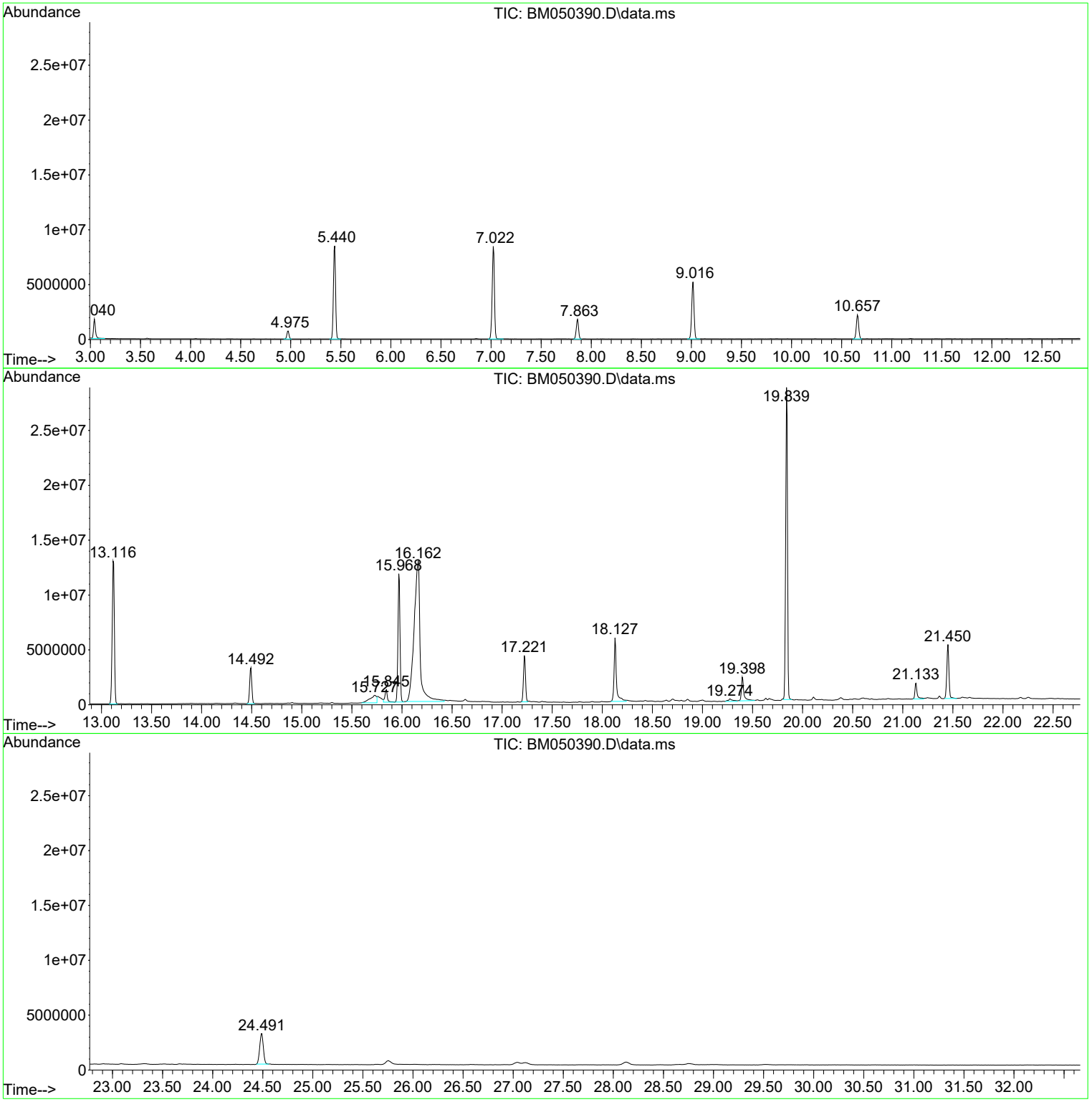
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-79

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM070925.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\BM071025\
Data File : BM050390.D
Acq On : 10 Jul 2025 15:17
Operator : RC/JU
Sample : Q2529-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM070925.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

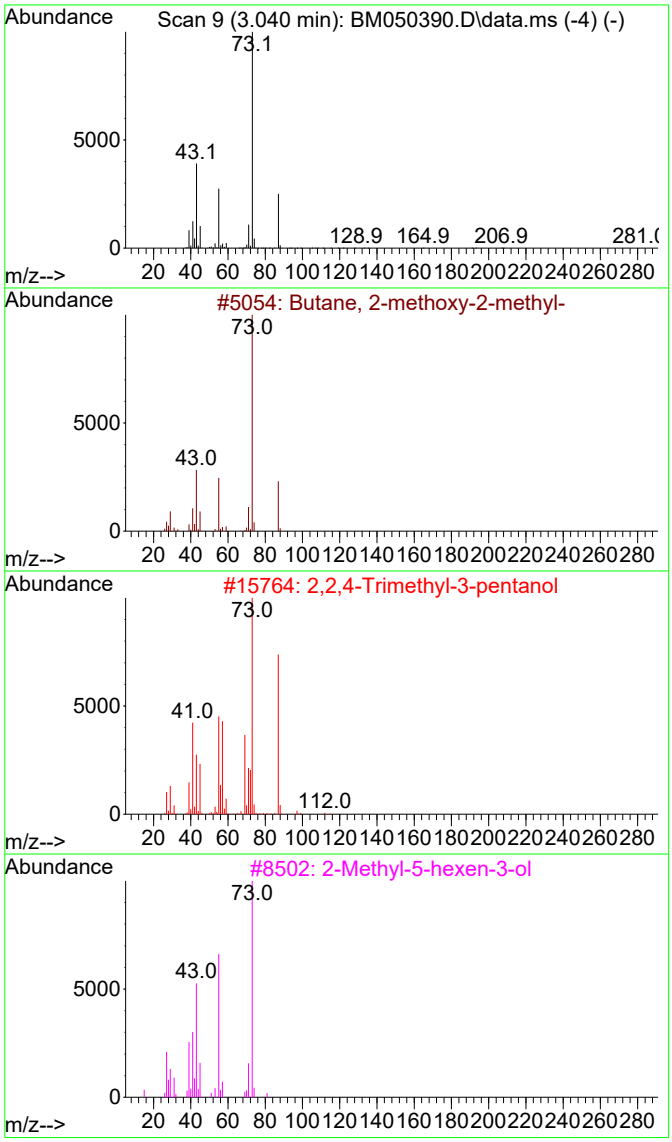
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

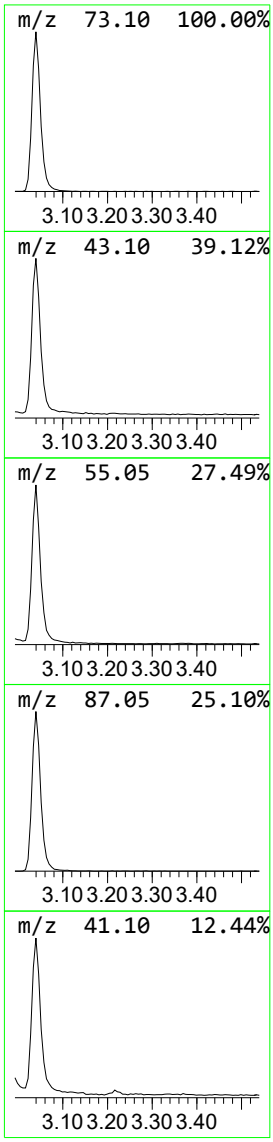
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.040	17.47 ng	2453880	1,4-Dichlorobenzene-d4	7.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	38
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25





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Data File : BM050390.D
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Operator : RC/JU
Sample : Q2529-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-79

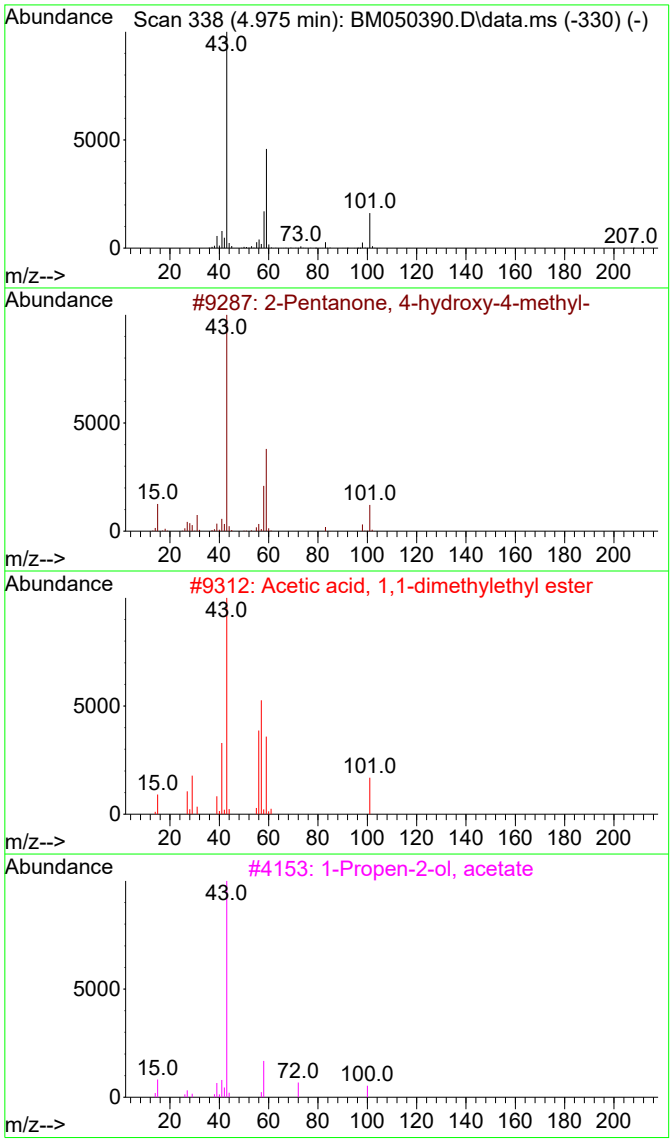
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM070925.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

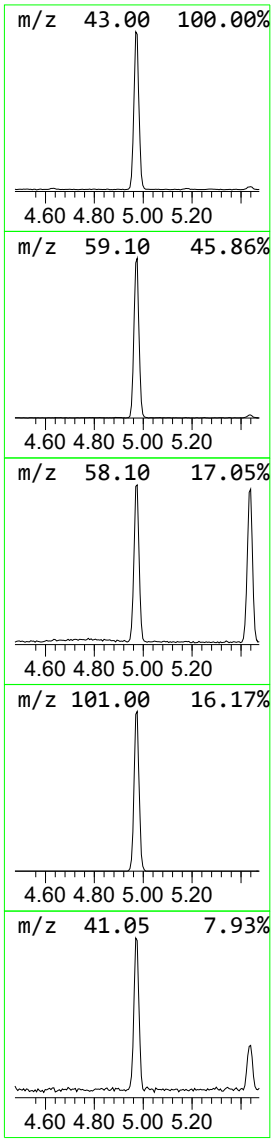
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.975	7.47 ng	1049420	1,4-Dichlorobenzene-d4	7.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
5	Butane	58	C4H10	000106-97-8	9





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Data File : BM050390.D
Acq On : 10 Jul 2025 15:17
Operator : RC/JU
Sample : Q2529-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-79

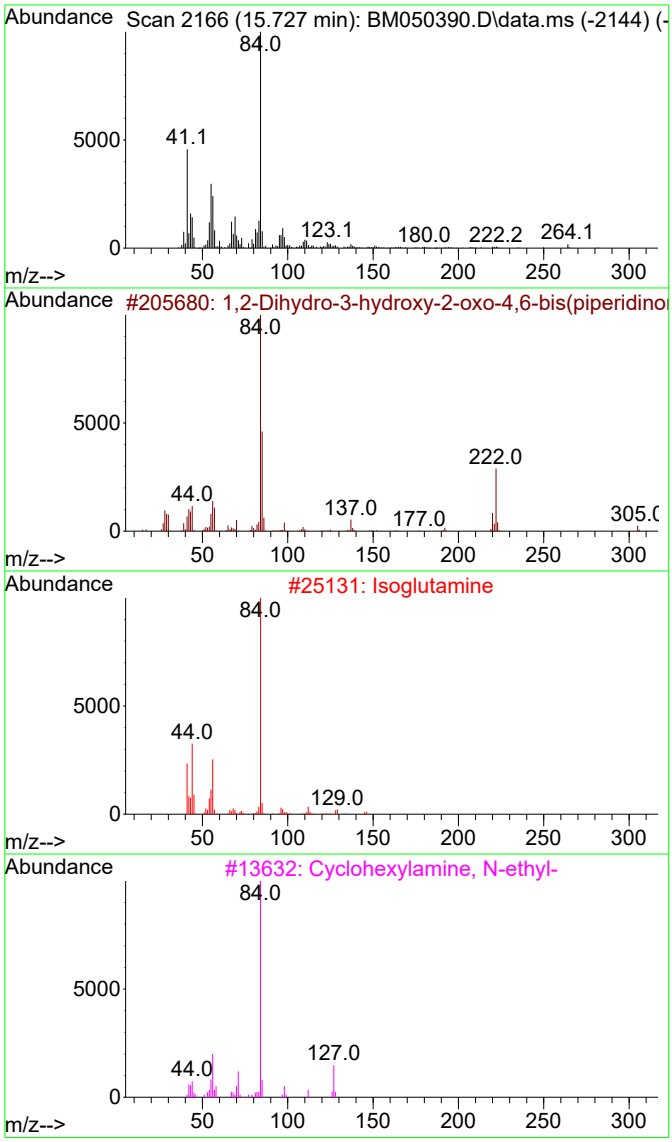
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM070925.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

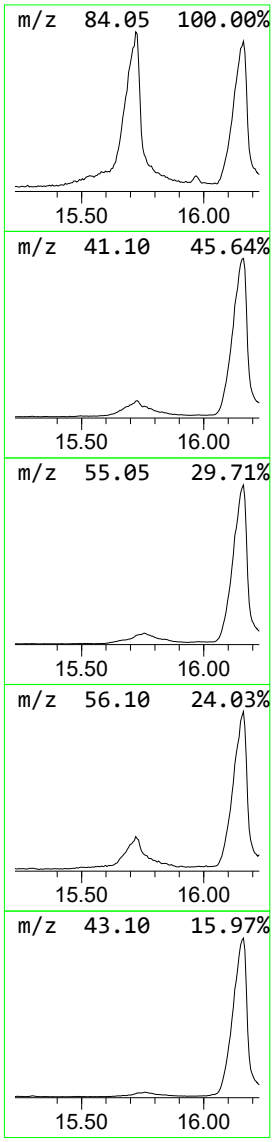
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1,2-Dihydro-3-hydroxy-2-oxo... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.727	13.16 ng	3191250	Acenaphthene-d10	14.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Dihydro-3-hydroxy-2-oxo-4,6-...	305	C17H27N3O2	020928-64-7	59
2	Isoglutamine	146	C5H10N2O3	000328-48-3	59
3	Cyclohexylamine, N-ethyl-	127	C8H17N	005459-93-8	59
4	1-(Piperidin-2-yl)ethan-1-ol, ac...	171	C9H17NO2	1000505-56-6	58
5	1,3,2-Dioxaborolan-4-one, 2-ethy...	128	C5H9BO3	074646-14-3	58





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Operator : RC/JU
Sample : Q2529-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-79

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM070925.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

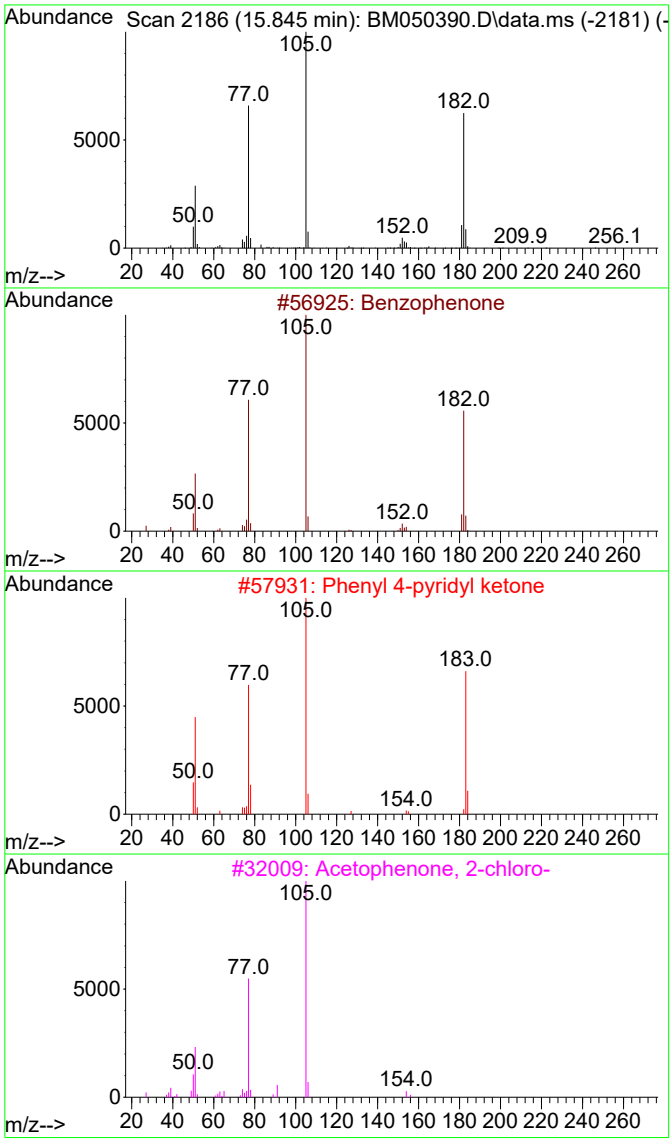
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

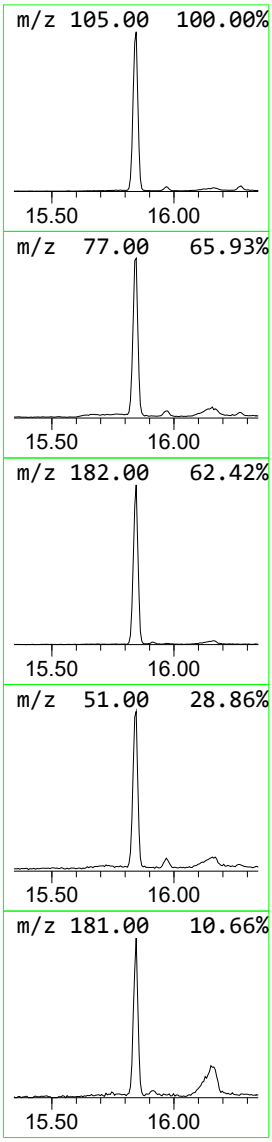
****

Peak Number 4 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.845	7.75 ng	1878520	Acenaphthene-d10	14.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	58
3	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
4	Benzoylformic acid	150	C8H6O3	000611-73-4	49
5	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM071025\
Data File : BM050390.D
Acq On : 10 Jul 2025 15:17
Operator : RC/JU
Sample : Q2529-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-79

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM070925.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

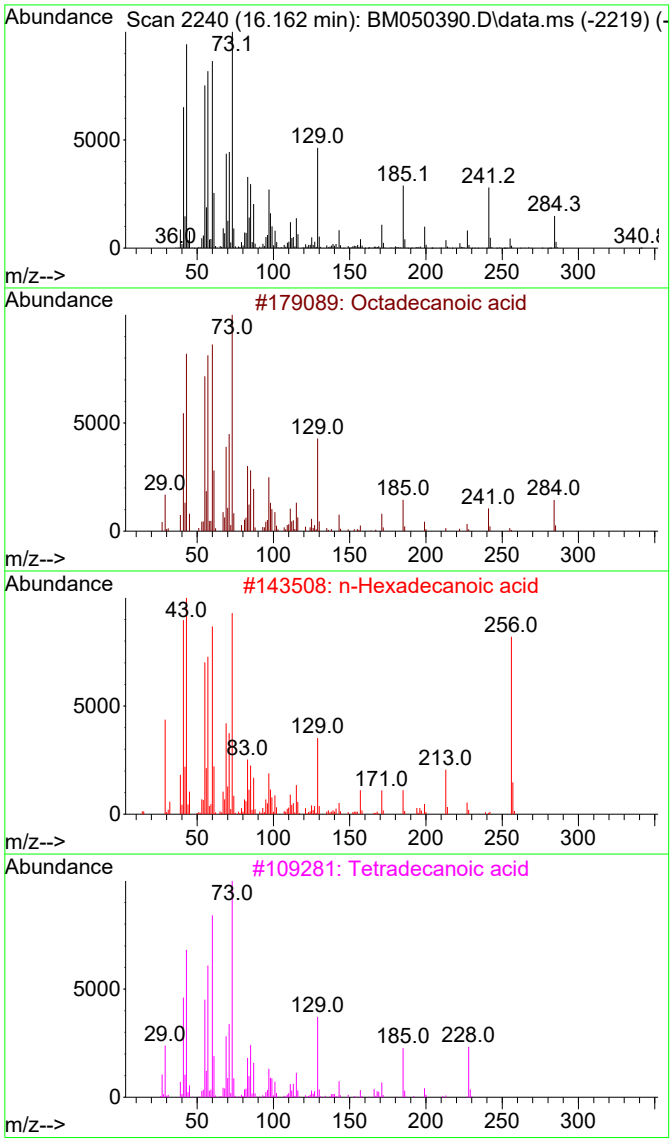
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

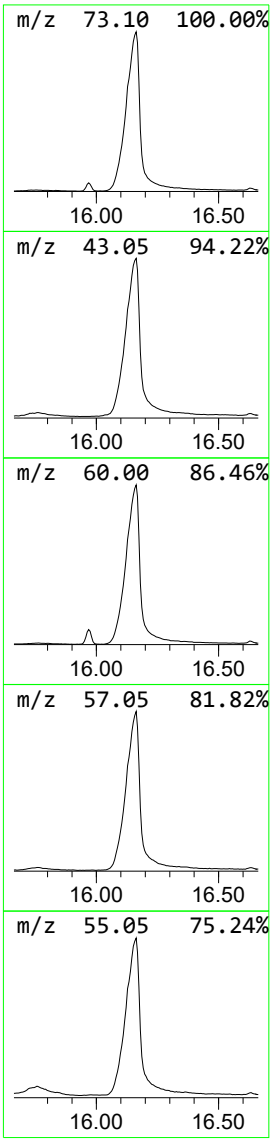
****

Peak Number 5 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.163	182.38 ng	54130900	Phenanthrene-d10	17.221

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	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





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Data File : BM050390.D
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Operator : RC/JU
Sample : Q2529-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-79

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM070925.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

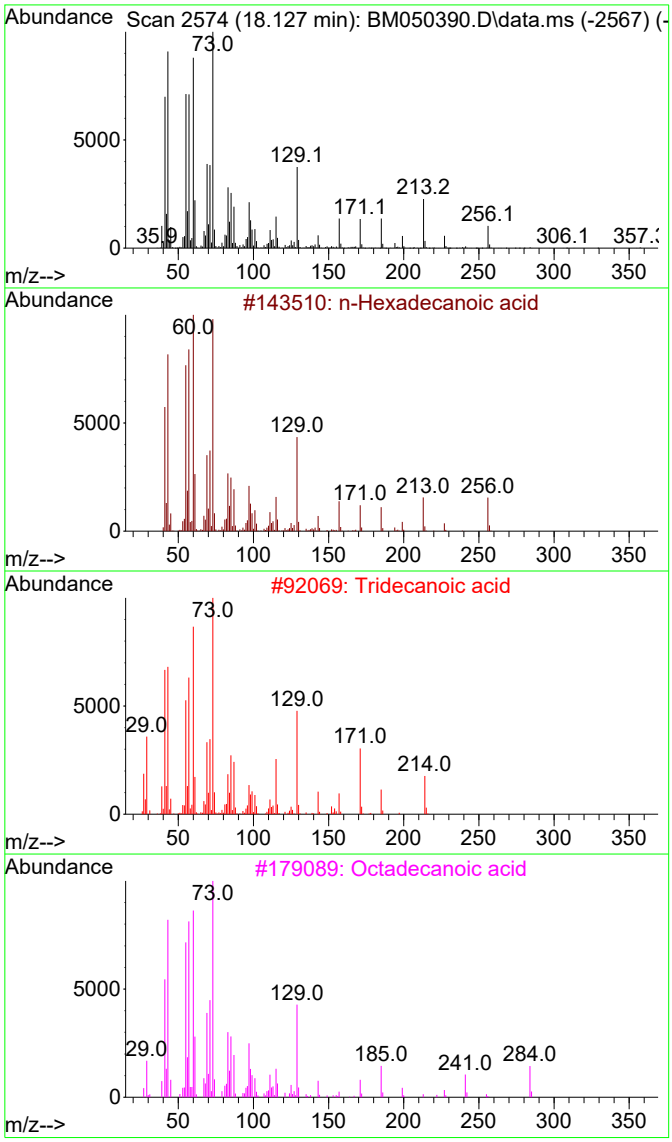
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

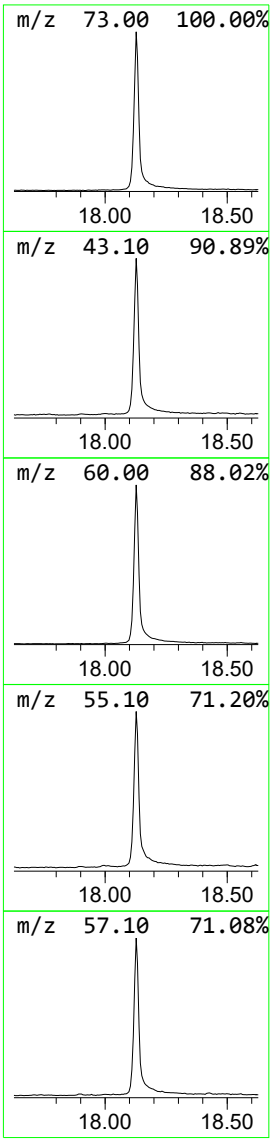
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.127	31.48 ng	9342100	Phenanthrene-d10	17.221

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	Octadecanoic acid	284	C18H36O2	000057-11-4	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	74





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM070925.M
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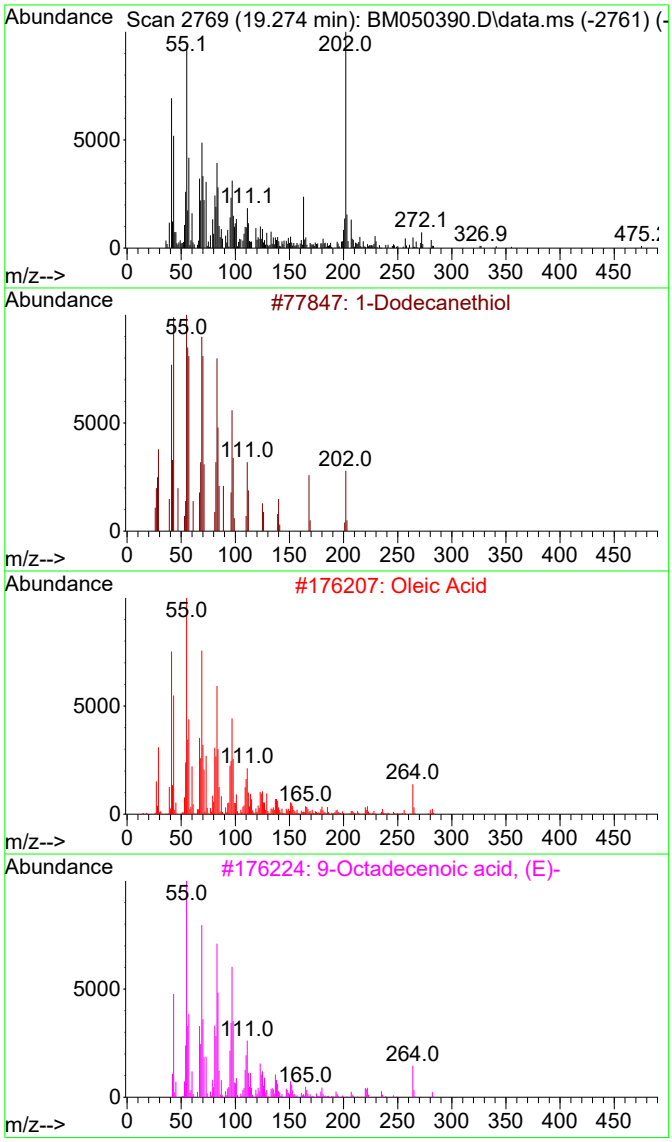
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

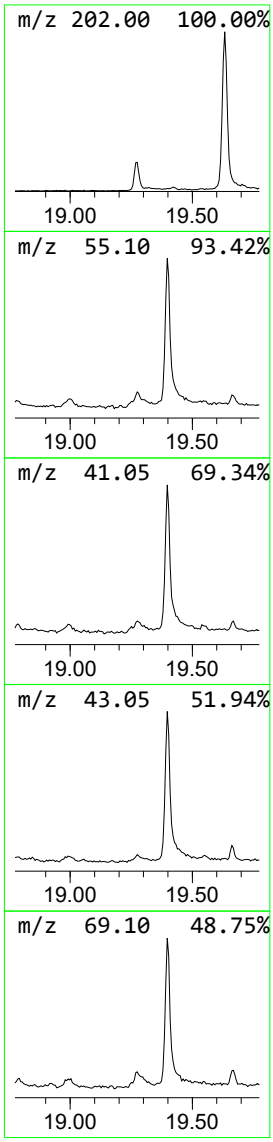
****

Peak Number 7 1-Dodecanethiol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.274	2.43 ng	721942	Phenanthrene-d10	17.221

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanethiol	202	C12H26S	000112-55-0	62
2	Oleic Acid	282	C18H34O2	000112-80-1	59
3	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	50
4	Pyrene	202	C16H10	000129-00-0	38
5	Fluoranthene	202	C16H10	000206-44-0	38





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Operator : RC/JU
Sample : Q2529-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM070925.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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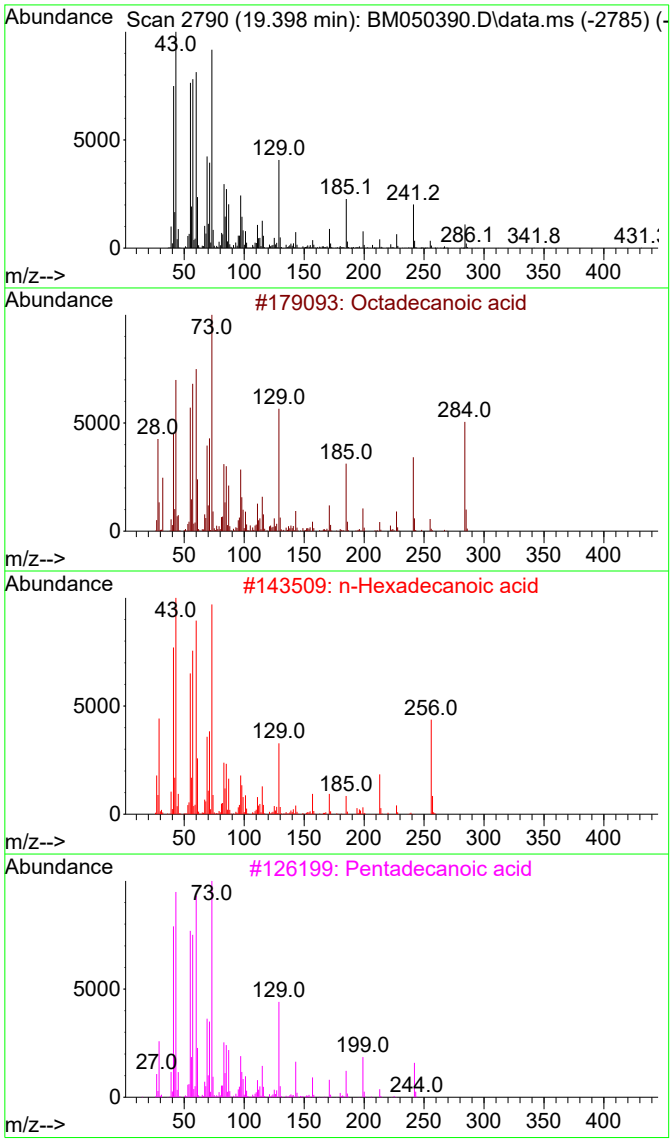
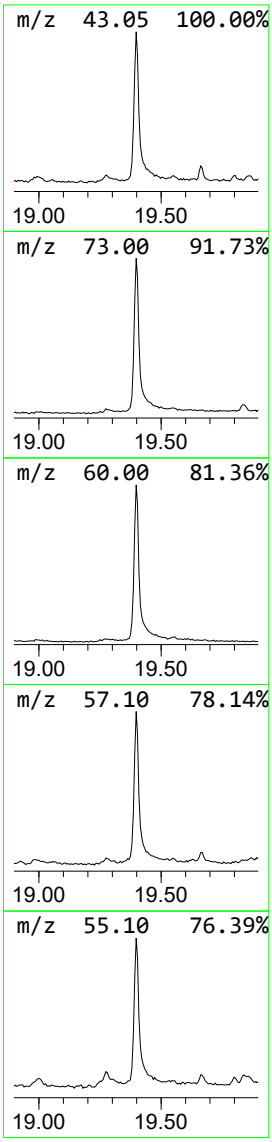
****

Peak Number 8 Pentadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.398	9.84 ng	3574090	Chrysene-d12	21.450

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	96
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	87





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BNA_M
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM070925.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

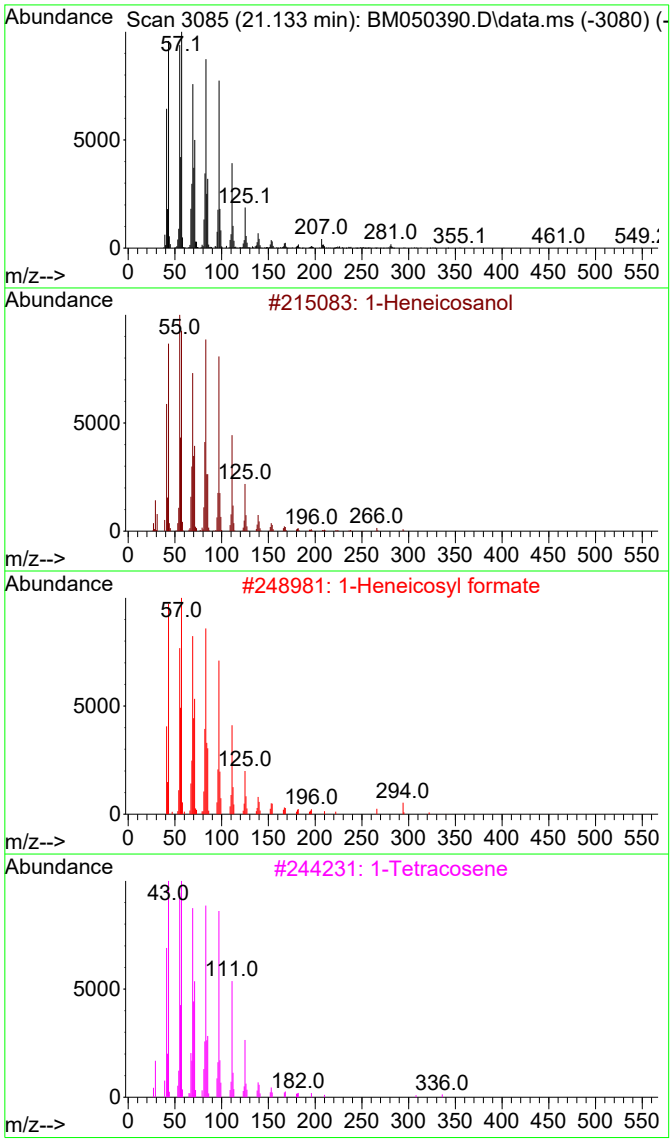
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

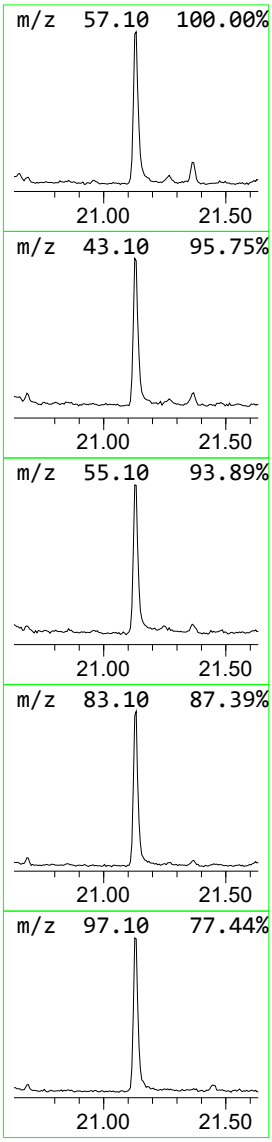
****

Peak Number 9 1-Heneicosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.133	6.24 ng	2264770	Chrysene-d12	21.450

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
3	1-Tetracosene	336	C24H48	010192-32-2	94
4	Pentacos-1-ene	350	C25H50	016980-85-1	94
5	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM071025\
Data File : BM050390.D
Acq On : 10 Jul 2025 15:17
Operator : RC/JU
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Misc :
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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM070925.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...	3.040	17.5	ng	2453880	1	7.863	2809230	20.0
2-Pentanone, 4-...	4.975	7.5	ng	1049420	1	7.863	2809230	20.0
1,2-Dihydro-3-h...	15.727	13.2	ng	3191250	3	14.492	4848230	20.0
Benzophenone	15.845	7.8	ng	1878520	3	14.492	4848230	20.0
Octadecanoic acid	16.163	182.4	ng	54130900	4	17.221	5936070	20.0
n-Hexadecanoic ...	18.127	31.5	ng	9342100	4	17.221	5936070	20.0
1-Dodecanethiol	19.274	2.4	ng	721942	4	17.221	5936070	20.0
Pentadecanoic acid	19.398	9.8	ng	3574090	5	21.450	7262450	20.0
1-Heneicosanol	21.133	6.2	ng	2264770	5	21.450	7262450	20.0