LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM020223\
Data File : BM038674.D
Acq On : 02 Feb 2023 21:47
Operator : CG/JU
Sample : 01348-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-H5(30.5-32)

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-BM020123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM038674.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.210	3	4	15	rVB	38122	46205	1.46%	0.260%
2	5.016	305	311	319	rBV	326404	449037	14.20%	2.527%
3	5.493	385	392	401	rBV	977713	1343910	42.49%	7.562%
4	6.469	551	558	571	rVB	28654	77653	2.46%	0.437%
5	7.110	660	667	678	rBV	857336	1304550	41.25%	7.340%
6	7.928	797	806	813	rBV	273449	409962	12.96%	2.307%
7	9.104	998	1006	1016	rBV	510938	811929	25.67%	4.568%
8	10.739	1277	1284	1289	rBV	294227	480929	15.21%	2.706%
9	13.192	1695	1701	1711	rVB	1750046	2347849	74.23%	13.211%
10	14.568	1928	1935	1945	rVB	468913	694341	21.95%	3.907%
11	15.274	2029	2055	2056	rBV2	54576	257266	8.13%	1.448%
12	15.927	2162	2166	2172	rVB2	22515	31839	1.01%	0.179%
13	16.057	2182	2188	2200	rBV	1325180	1775970	56.15%	9.993%
14	17.309	2395	2401	2407	rBV	585269	788777	24.94%	4.438%
15	18.198	2547	2552	2562	rBV	172898	257857	8.15%	1.451%
16	19.468	2764	2768	2776	rBV	70435	102541	3.24%	0.577%
17	19.927	2841	2846	2852	rBV	2831532	3162859	100.00%	17.796%
18	20.139	2877	2882	2887	rBV	864174	991699	31.35%	5.580%
19	20.609	2958	2962	2969	rBV	141863	183457	5.80%	1.032%
20	21.180	3055	3059	3069	rBV2	144297	208156	6.58%	1.171%
21	21.386	3091	3094	3098	rBV	140608	139844	4.42%	0.787%
22	21.486	3106	3111	3119	rBV	687728	880869	27.85%	4.956%
23	23.885	3513	3519	3532	rVB2	520581	1024896	32.40%	5.767%

Sum of corrected areas: 17772395

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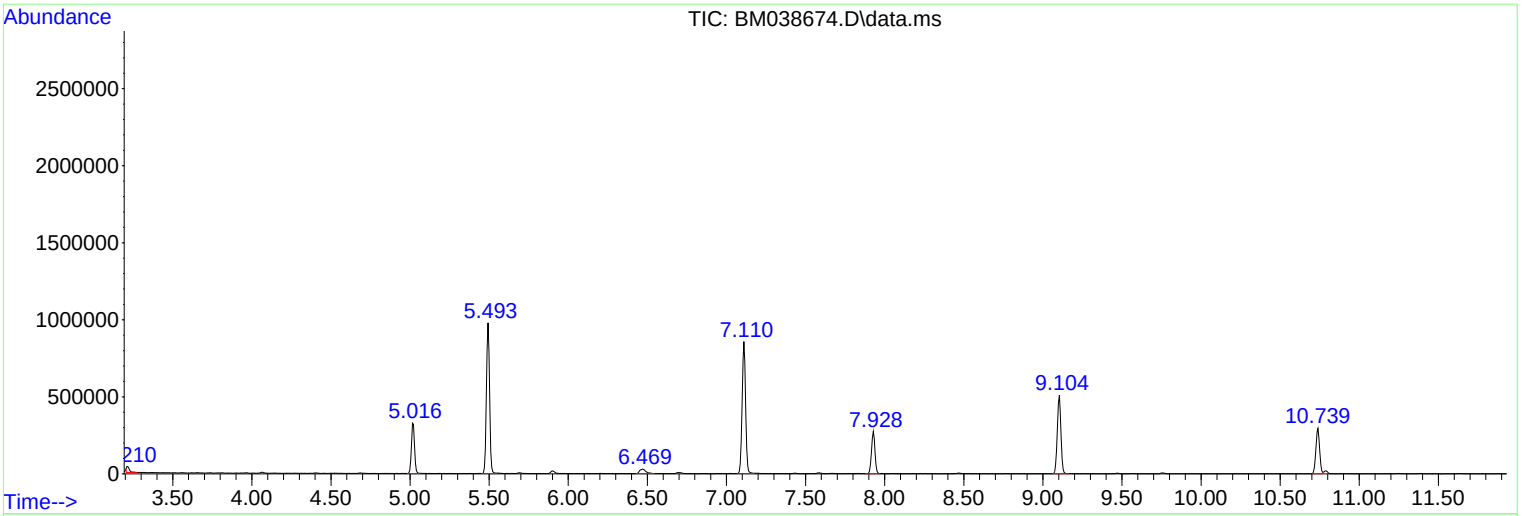
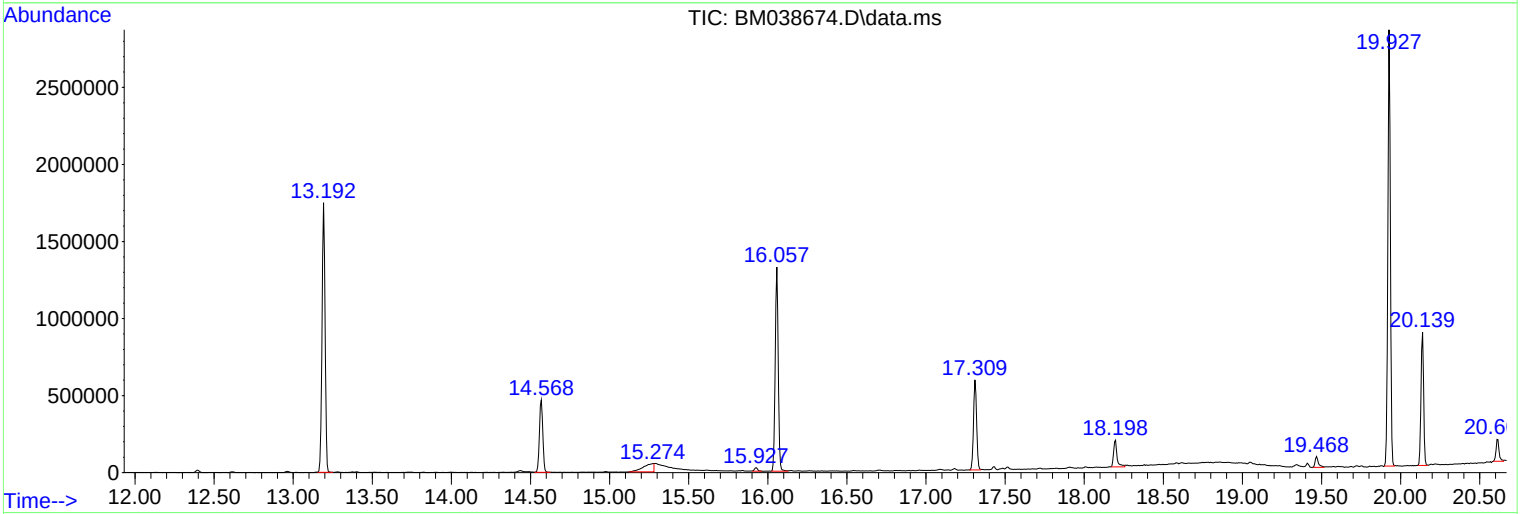
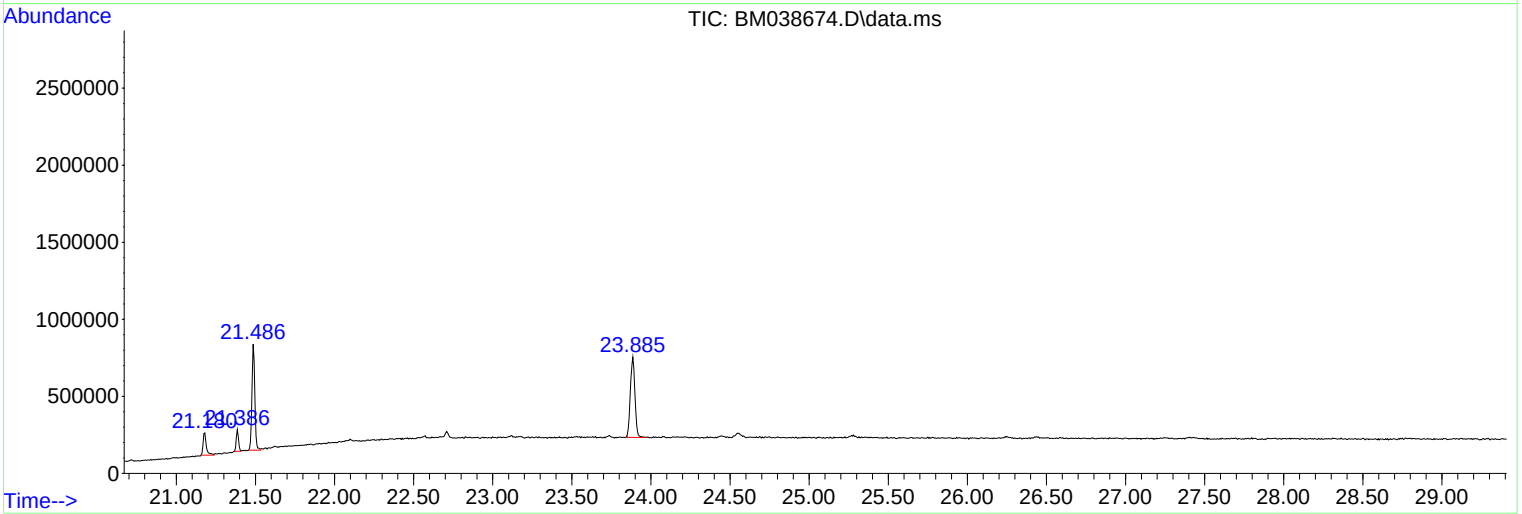
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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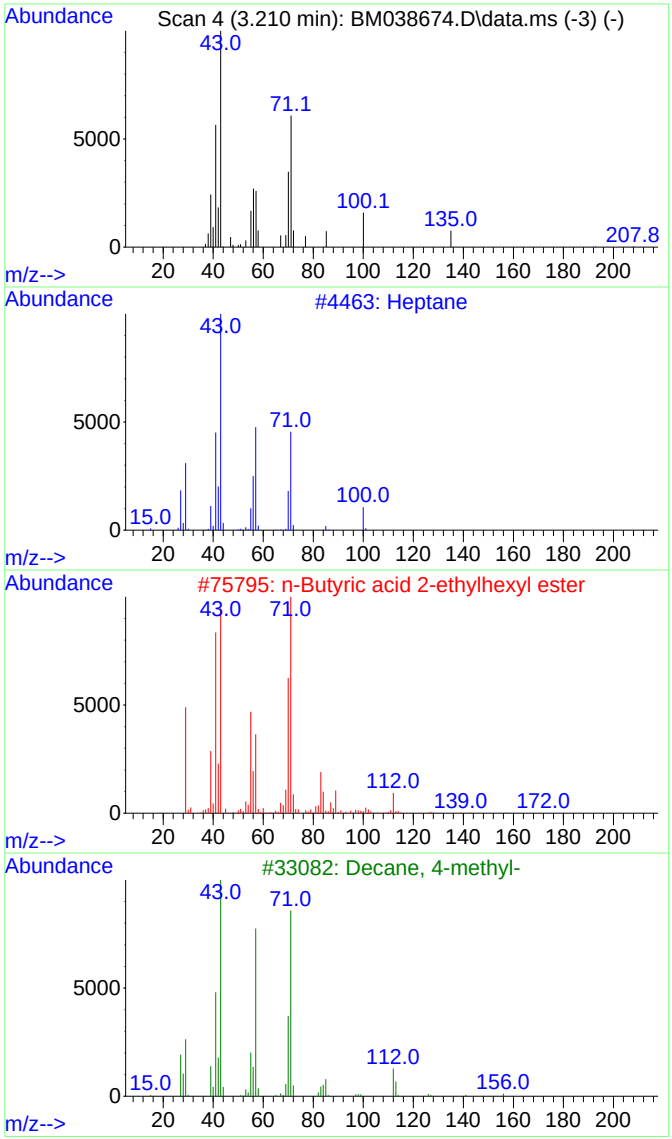
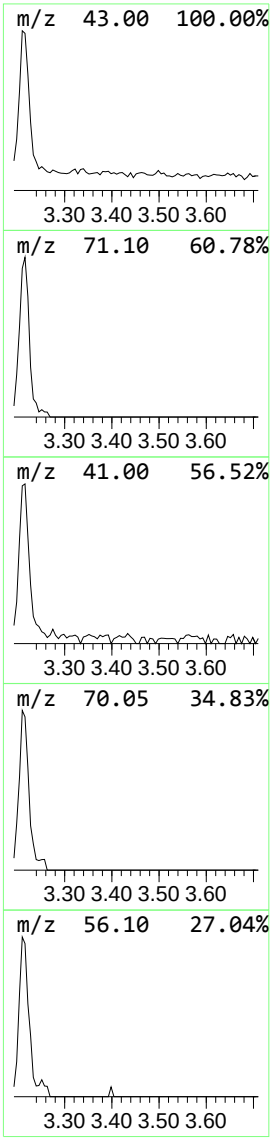
Peak Number 1 Heptane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.210	2.25 ng	46205	1,4-Dichlorobenzene-d4	7.928

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane	100	C7H16	000142-82-5	72
2	n-Butyric acid 2-ethylhexyl ester	200	C12H24O2	025415-84-3	50
3	Decane, 4-methyl-	156	C11H24	002847-72-5	45
4	Octane, 3,3-dimethyl-	142	C10H22	004110-44-5	40
5	Butanoic acid, 2-bromo-, 1-methy...	236	C9H17BrO2	1000131-81-9	40





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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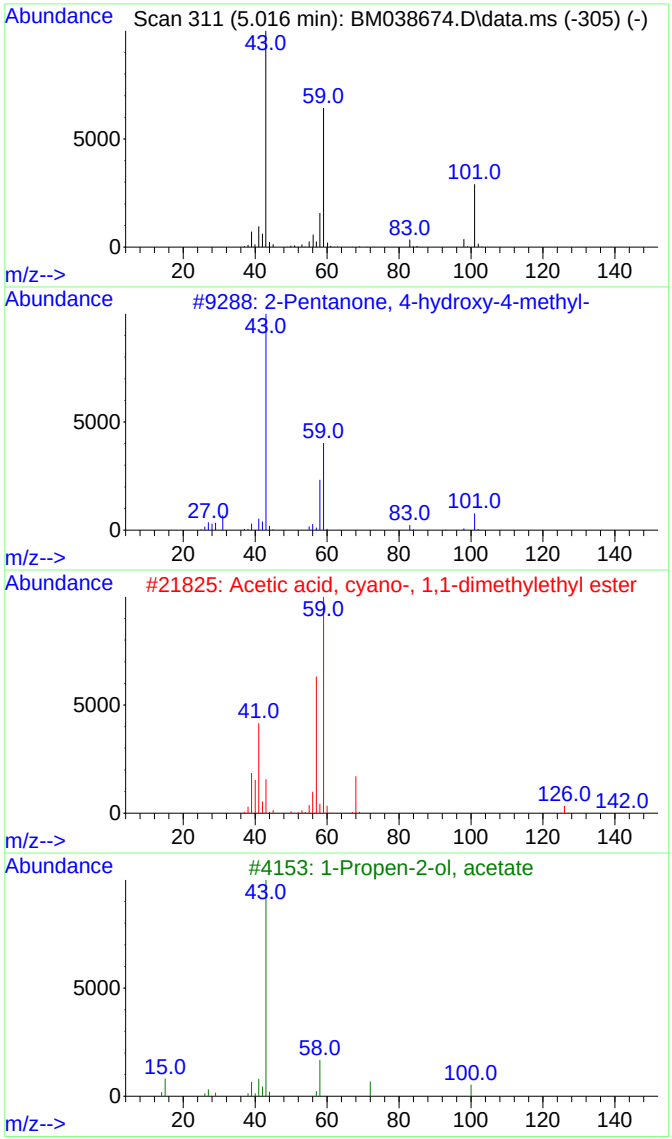
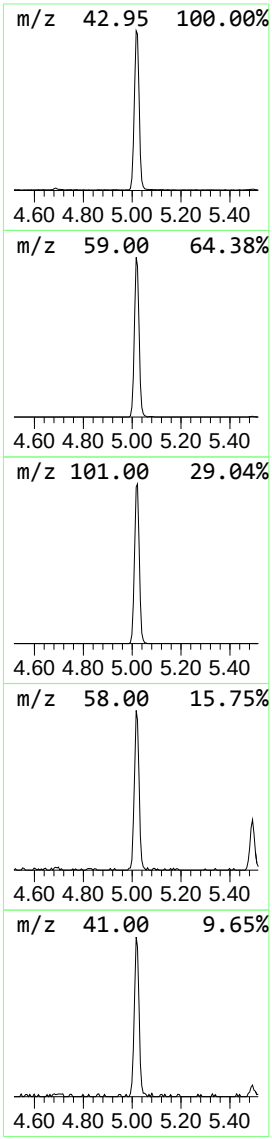
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.016	21.91 ng	449037	1,4-Dichlorobenzene-d4	7.928

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Acetone	58	C3H6O	000067-64-1	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





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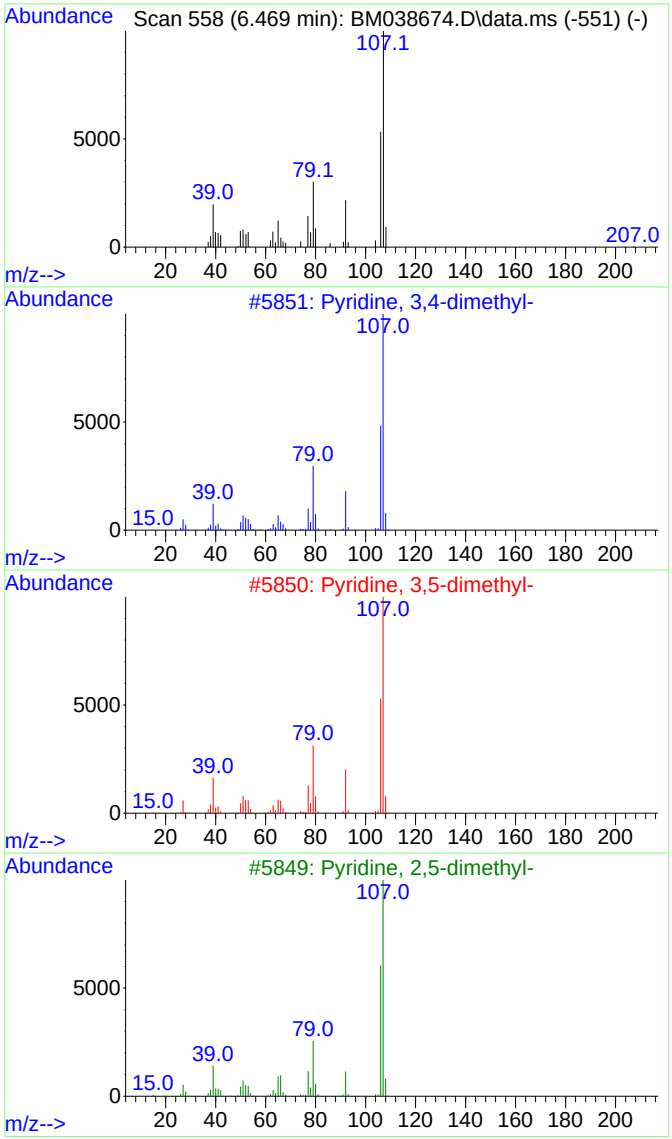
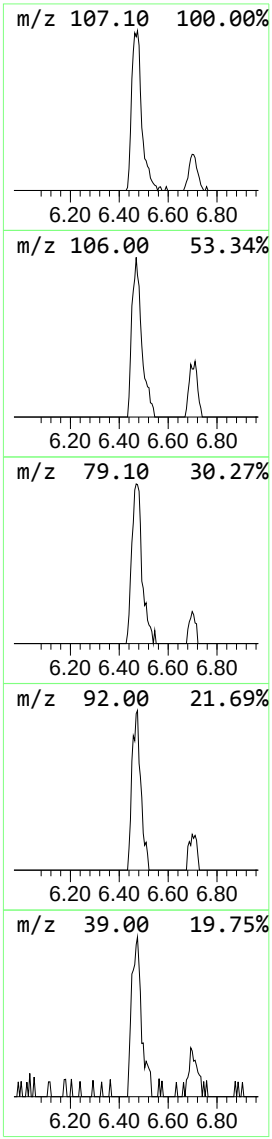
Peak Number 3 Pyridine, 3,4-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.469	3.79 ng	77653	1,4-Dichlorobenzene-d4	7.928

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyridine, 3,4-dimethyl-	107	C7H9N	000583-58-4	96
2	Pyridine, 3,5-dimethyl-	107	C7H9N	000591-22-0	94
3	Pyridine, 2,5-dimethyl-	107	C7H9N	000589-93-5	93
4	Pyridine, 2,4-dimethyl-	107	C7H9N	000108-47-4	91
5	Pyridine, 2,3-dimethyl-	107	C7H9N	000583-61-9	74





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S-H5(30.5-32)

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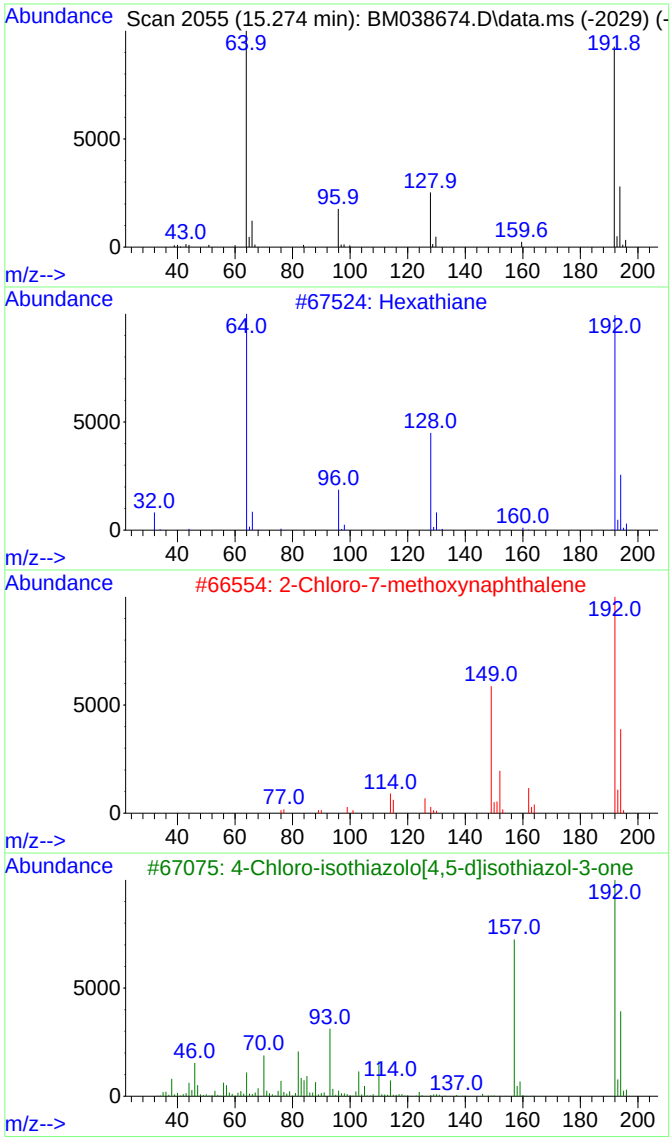
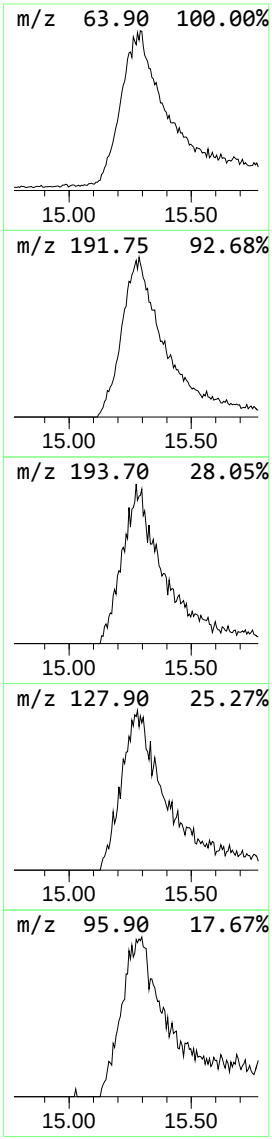
Peak Number 4 Hexathiane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.274	7.41 ng	257266	Acenaphthene-d10	14.568

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexathiane	192	S6	013798-23-7	91
2	2-Chloro-7-methoxynaphthalene	192	C11H9ClO	067061-67-0	36
3	4-Chloro-isothiazolo[4,5-d]isoth...	192	C4HClN2OS2	1000274-74-8	11
4	Pyrazole, 3-(p-chlorophenyl)-5-m...	192	C10H9ClN2	017629-27-5	10
5	Benzene, 1-bromo-4-chloro-	190	C6H4BrCl	000106-39-8	9





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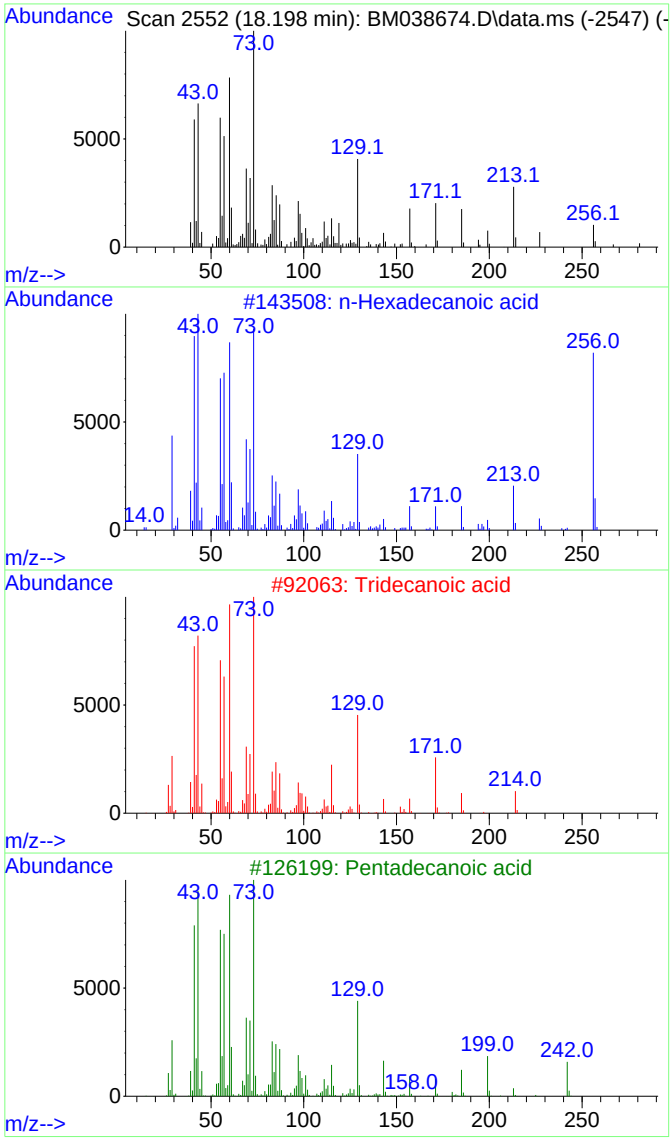
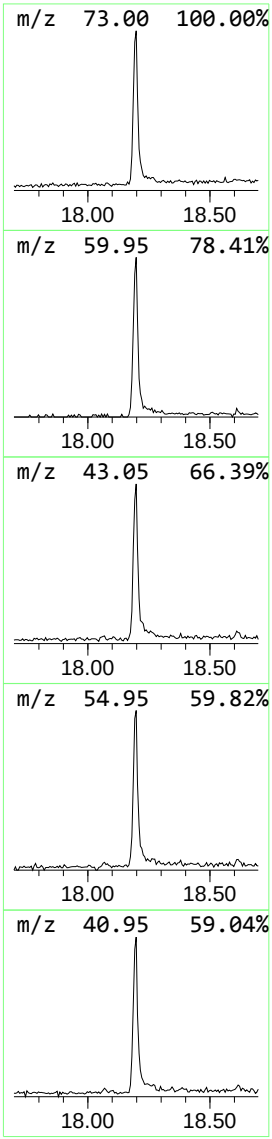
Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.198	6.54 ng	257857	Phenanthrene-d10	17.309

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4	n-Decanoic acid	172	C10H20O2	000334-48-5	64
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





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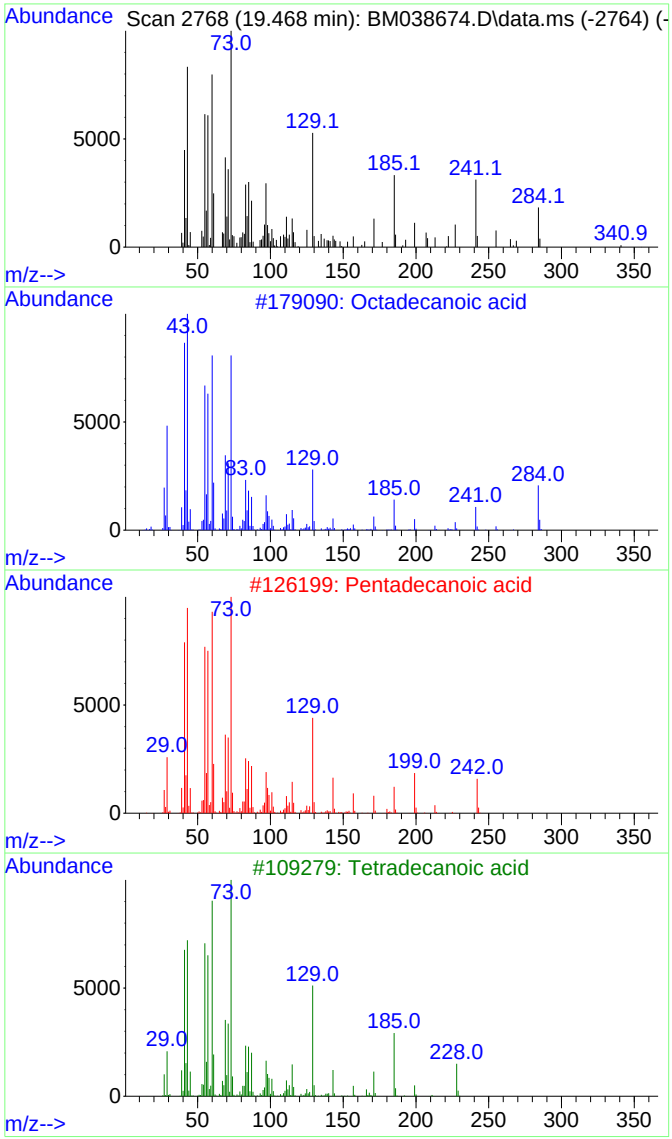
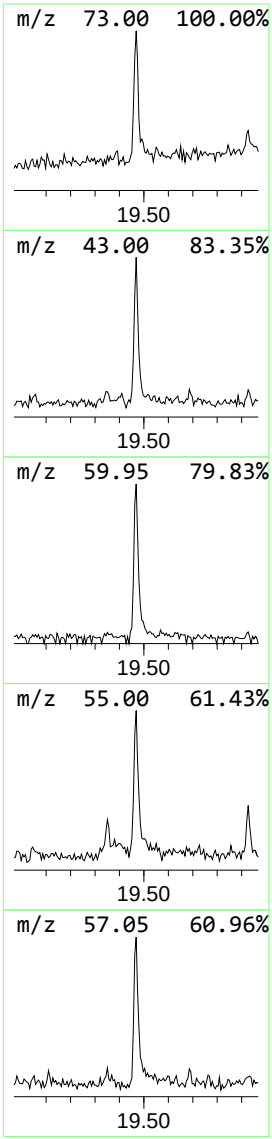
Peak Number 6 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.468	2.33 ng	102541	Chrysene-d12	21.486

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	52





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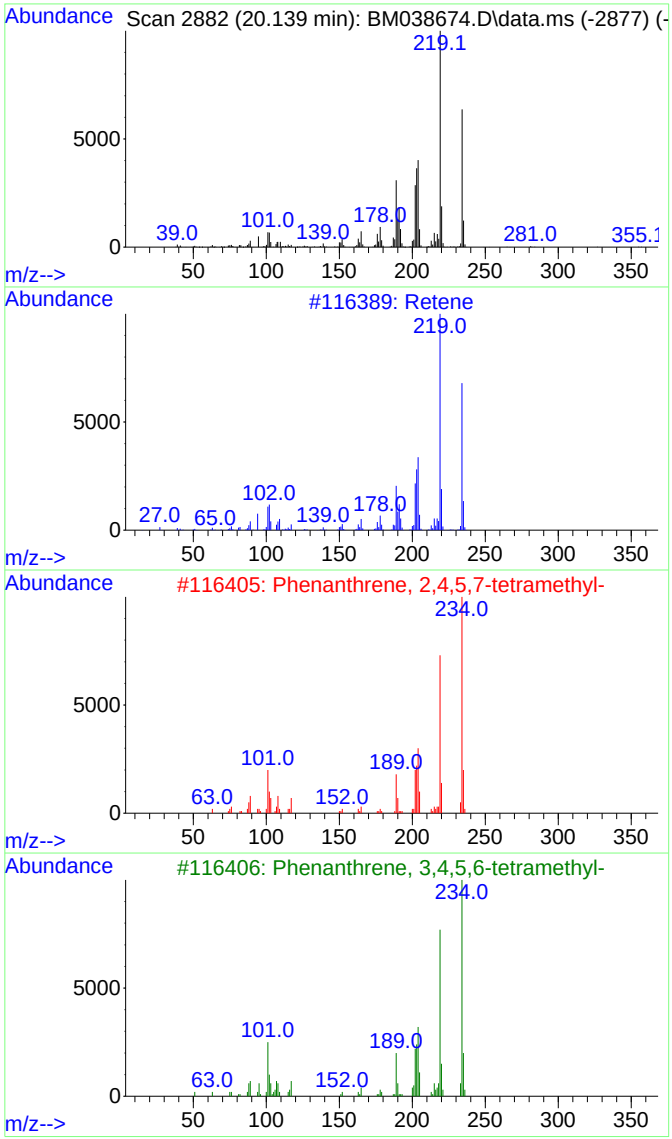
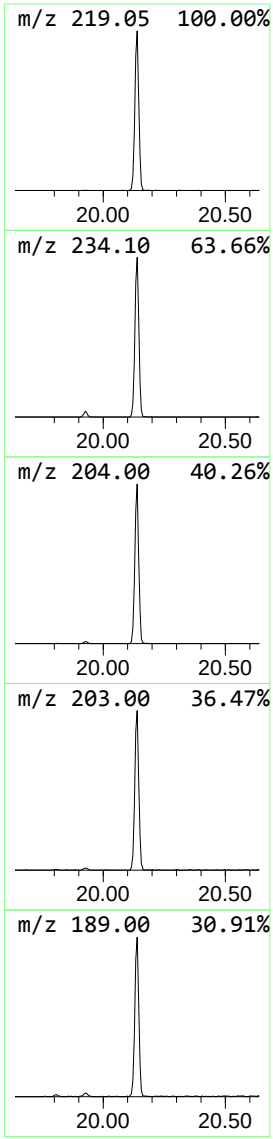
Peak Number 7 Retene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.139	22.52 ng	991699	Chrysene-d12	21.486

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Retene	234	C18H18	000483-65-8	98
2	Phenanthrene, 2,4,5,7-tetramethyl-	234	C18H18	007396-38-5	94
3	Phenanthrene, 3,4,5,6-tetramethyl-	234	C18H18	007343-06-8	94
4	2-Isopropyl-10-methylphenanthrene	234	C18H18	066552-97-4	93
5	1,4-Di-(4'-methylphenyl)buta-1,3...	234	C18H18	1000202-17-5	72





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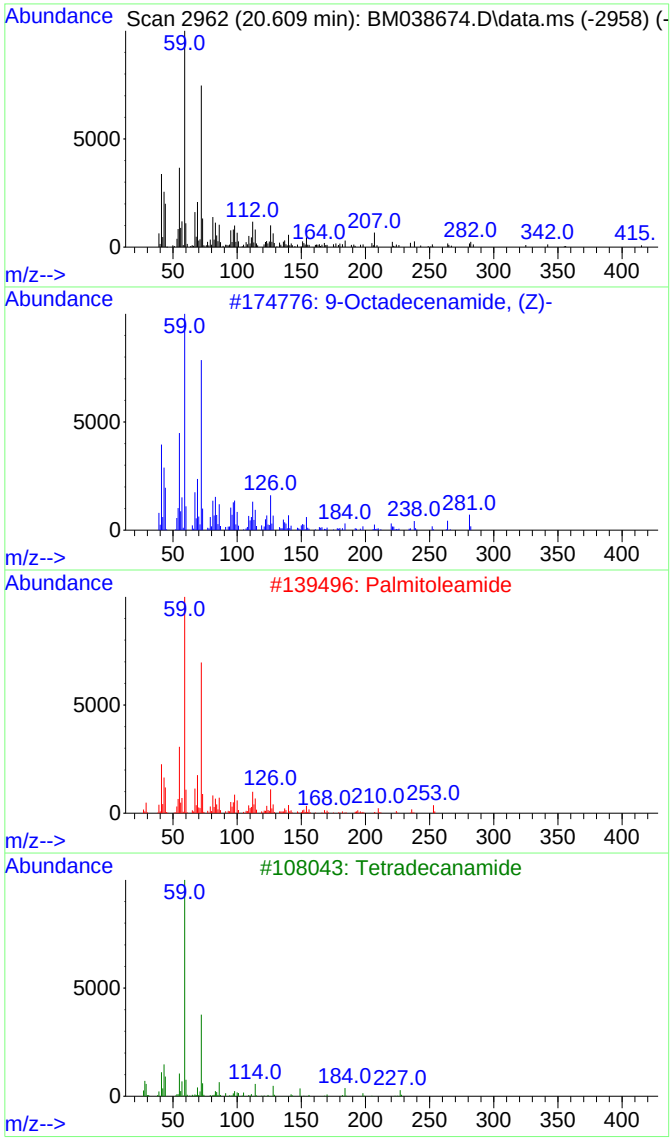
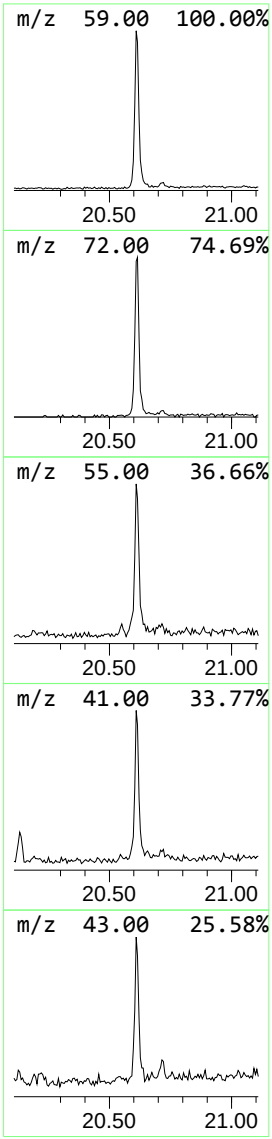
Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.609	4.17 ng	183457	Chrysene-d12	21.486

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	97
2	Palmitoleamide	253	C16H31NO	106010-22-4	72
3	Tetradecanamide	227	C14H29NO	000638-58-4	43
4	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	35
5	N,N-Dimethyl cyanoacetamide	112	C5H8N2O	007391-40-4	27





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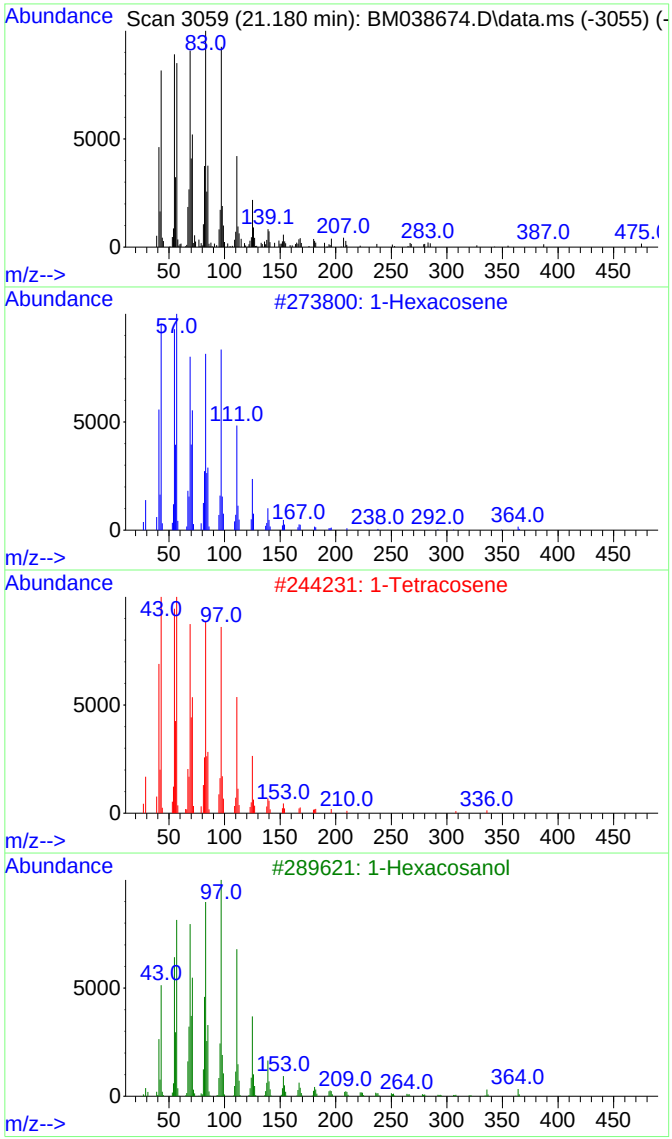
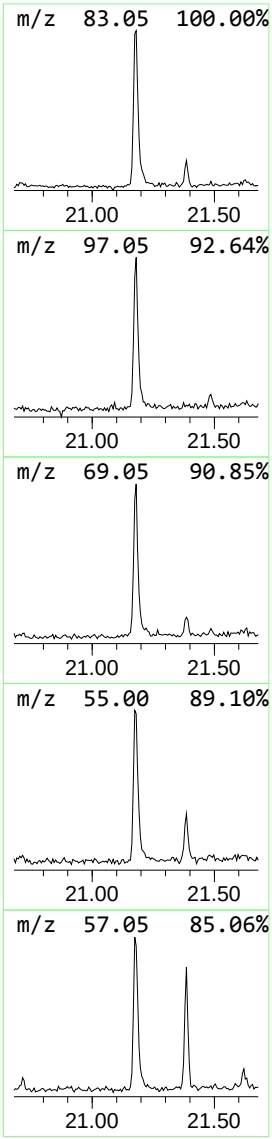
Peak Number 9 1-Hexacosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.180	4.73 ng	208156	Chrysene-d12	21.486

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene	364	C26H52	018835-33-1	95
2	1-Tetracosene	336	C24H48	010192-32-2	95
3	1-Hexacosanol	382	C26H54O	000506-52-5	94
4	1-Heptacosanol	396	C27H56O	002004-39-9	93
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	93





Tentatively Identified Compound (LSC) summary

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Data File : BM038674.D
Acq On : 02 Feb 2023 21:47
Operator : CG/JU
Sample : 01348-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-H5(30.5-32)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.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
Heptane	3.210	2.3	ng	46205	1	7.928	409962	20.0
2-Pentanone, 4-...	5.016	21.9	ng	449037	1	7.928	409962	20.0
Pyridine, 3,4-d...	6.469	3.8	ng	77653	1	7.928	409962	20.0
Hexathiane	15.274	7.4	ng	257266	3	14.568	694341	20.0
n-Hexadecanoic ...	18.198	6.5	ng	257857	4	17.309	788777	20.0
Octadecanoic acid	19.468	2.3	ng	102541	5	21.486	880869	20.0
Retene	20.139	22.5	ng	991699	5	21.486	880869	20.0
9-Octadecenamid...	20.609	4.2	ng	183457	5	21.486	880869	20.0
1-Hexacosene	21.180	4.7	ng	208156	5	21.486	880869	20.0