LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030821\
Data File : BM029024.D
Acq On : 08 Mar 2021 18:19
Operator : CG/JU
Sample : M1575-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : IDW-GW807B-AQ-030421

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: BM029024.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.246	379	384	393	rBB	81924	113054	18.43%	4.597%
2	5.722	460	465	470	rBV2	11469	16125	2.63%	0.656%
3	6.869	654	660	669	rBB	45849	72309	11.79%	2.940%
4	7.669	791	796	802	rBB	37585	54522	8.89%	2.217%
5	8.304	898	904	910	rBB2	4363	7118	1.16%	0.289%
6	8.845	990	996	1005	rVB	101562	159552	26.02%	6.487%
7	9.887	1168	1173	1184	rVB2	6255	10256	1.67%	0.417%
8	10.463	1265	1271	1278	rBV	47118	74172	12.09%	3.016%
9	11.286	1405	1411	1416	rBV2	3995	6376	1.04%	0.259%
10	11.363	1420	1424	1433	rVB	7384	12144	1.98%	0.494%
11	12.951	1688	1694	1702	rVB	239727	330891	53.95%	13.453%
12	14.222	1902	1910	1917	rBV3	3099	7909	1.29%	0.322%
13	14.339	1924	1930	1935	rVB2	62920	87777	14.31%	3.569%
14	15.839	2179	2185	2192	rBV	199708	280452	45.73%	11.403%
15	17.086	2391	2397	2402	rBV	76272	101663	16.58%	4.133%
16	17.980	2543	2549	2558	rBV	41399	54506	8.89%	2.216%
17	18.721	2670	2675	2679	rVB	20001	22473	3.66%	0.914%
18	19.262	2763	2767	2775	rBV2	23698	29663	4.84%	1.206%
19	19.709	2838	2843	2848	rBV	523099	613295	100.00%	24.936%
20	20.221	2924	2930	2940	rBV	53704	82739	13.49%	3.364%
21	20.974	3053	3058	3063	rBV	46753	56862	9.27%	2.312%
22	21.256	3102	3106	3111	rBV	107800	129539	21.12%	5.267%
23	23.415	3467	3473	3482	rVB2	78640	136125	22.20%	5.535%

Sum of corrected areas: 2459522

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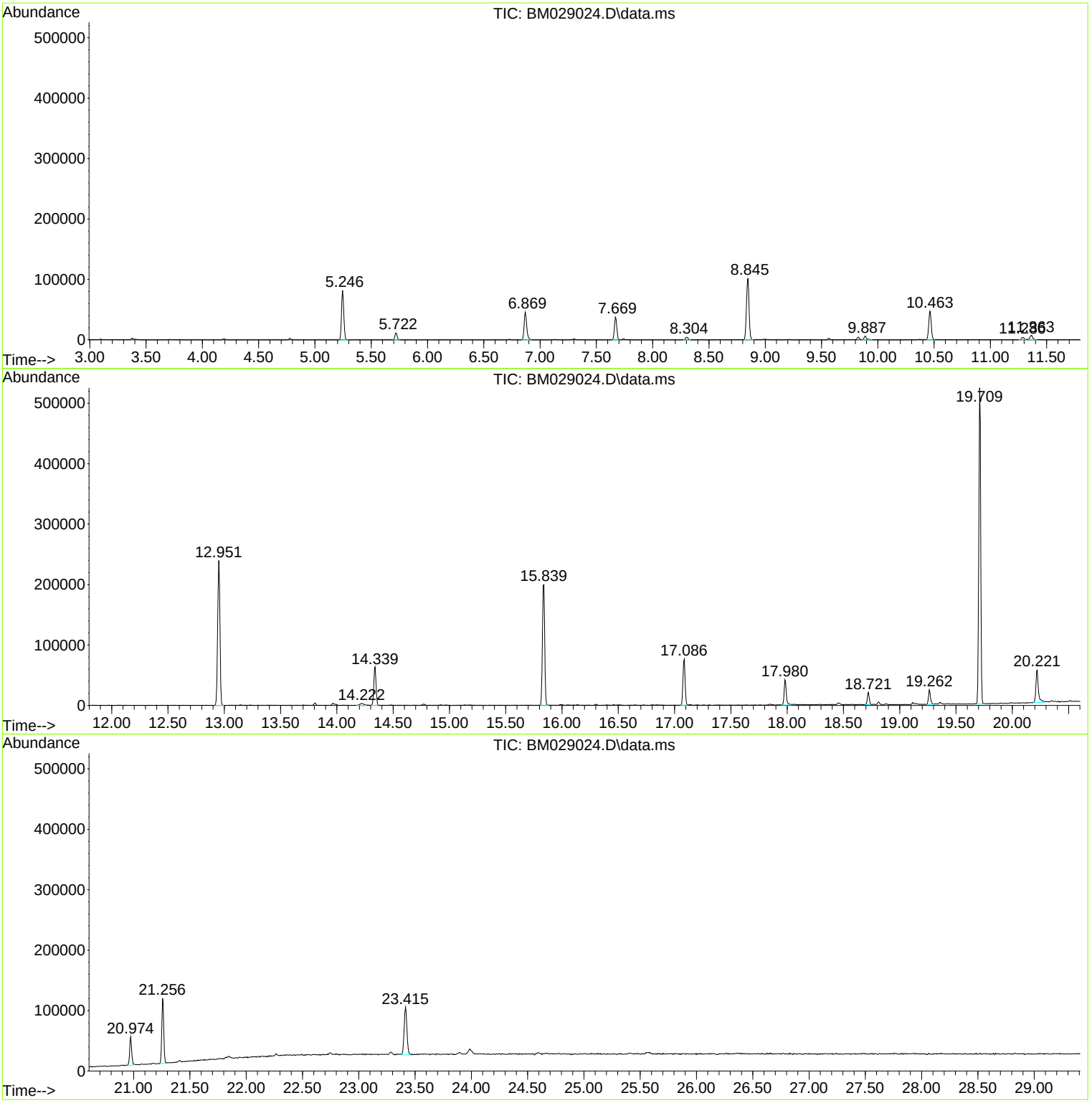
IDW-GW807B-AQ-030421

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



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TIC Library : C:\DATABASE\NIST11.L
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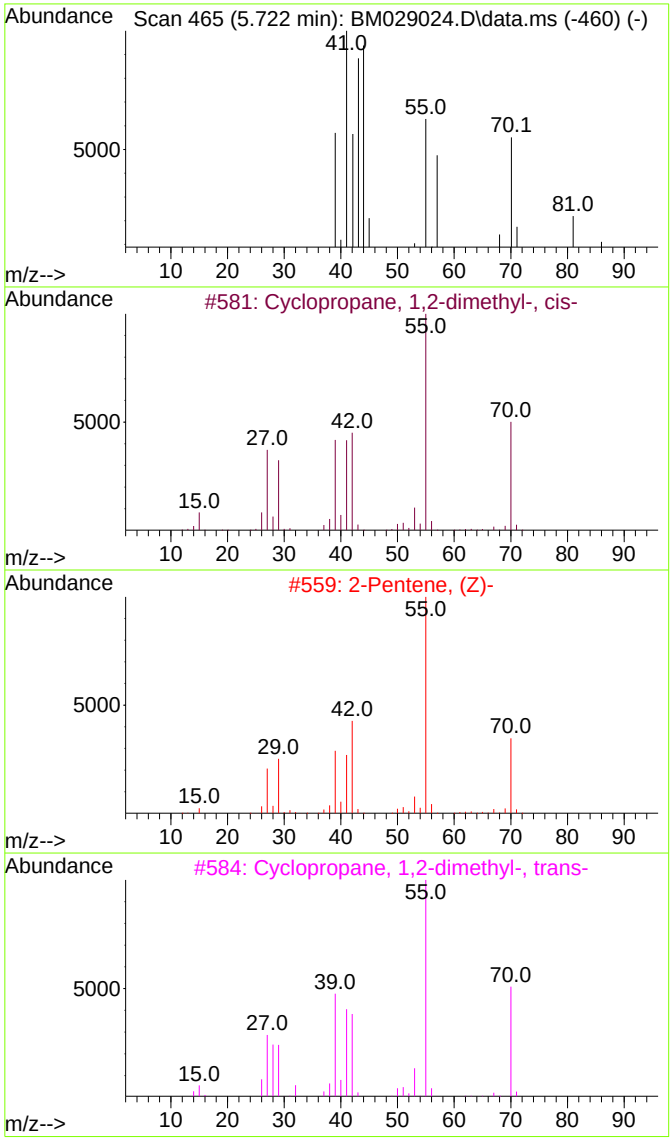
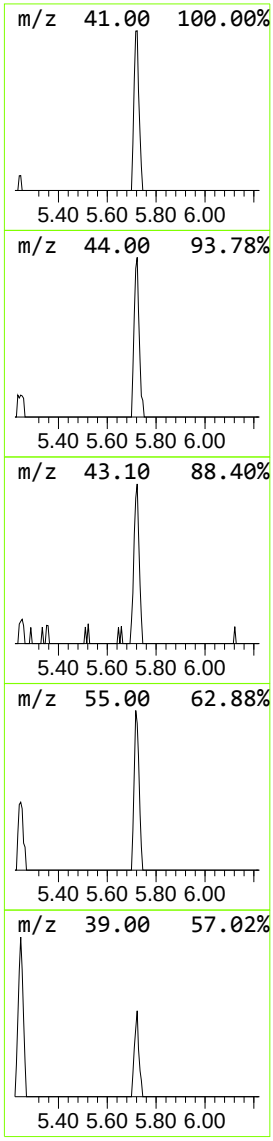
Peak Number 1 unknown5.722 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.722	5.92 ng	16125	1,4-Dichlorobenzene-d4	7.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	35
2	2-Pentene, (Z)-	70	C5H10	000627-20-3	25
3	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	25
4	Diaziridine,1,3,3-trimethyl-	86	C4H10N2	040711-15-7	23
5	2-Methyl-1-butene	70	C5H10	000563-46-2	17





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Instrument : BNA_M
ClientSampleId : IDW-GW807B-AQ-030421

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
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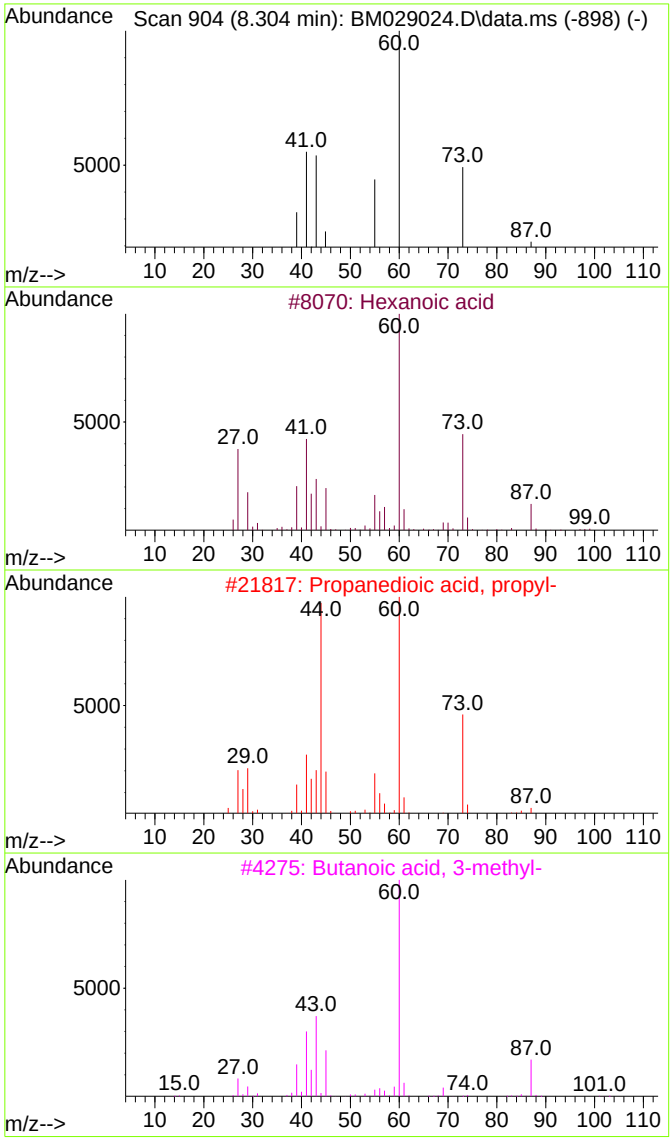
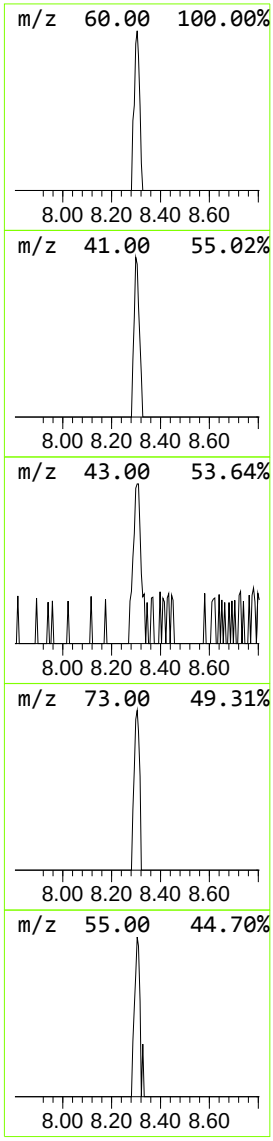
Peak Number 2 unknown8.304 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.304	2.61 ng	7118	1,4-Dichlorobenzene-d4	7.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid	116	C6H12O2	000142-62-1	40
2	Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	9
3	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	9
4	Isobutylamine	73	C4H11N	000078-81-9	5
5	1-Butanamine, 2-methyl-	87	C5H13N	000096-15-1	5





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BNA_M
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IDW-GW807B-AQ-030421

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
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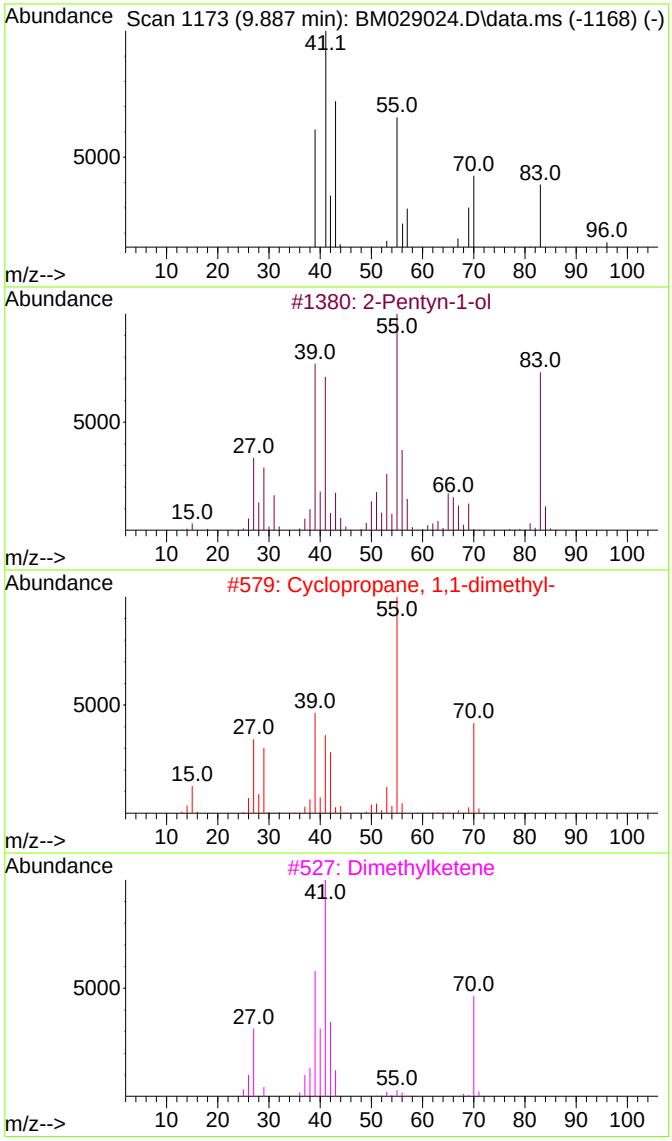
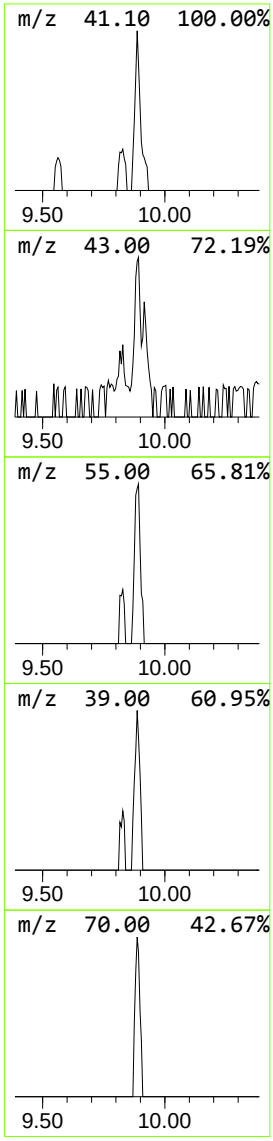
Peak Number 3 unknown9.887 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.887	2.77 ng	10256	Naphthalene-d8	10.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentyn-1-ol	84	C5H8O	006261-22-9	38
2	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	37
3	Dimethylketene	70	C4H6O	000598-26-5	32
4	1-Butene, 3-methyl-	70	C5H10	000563-45-1	25
5	4-Pentenal	84	C5H8O	002100-17-6	23





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

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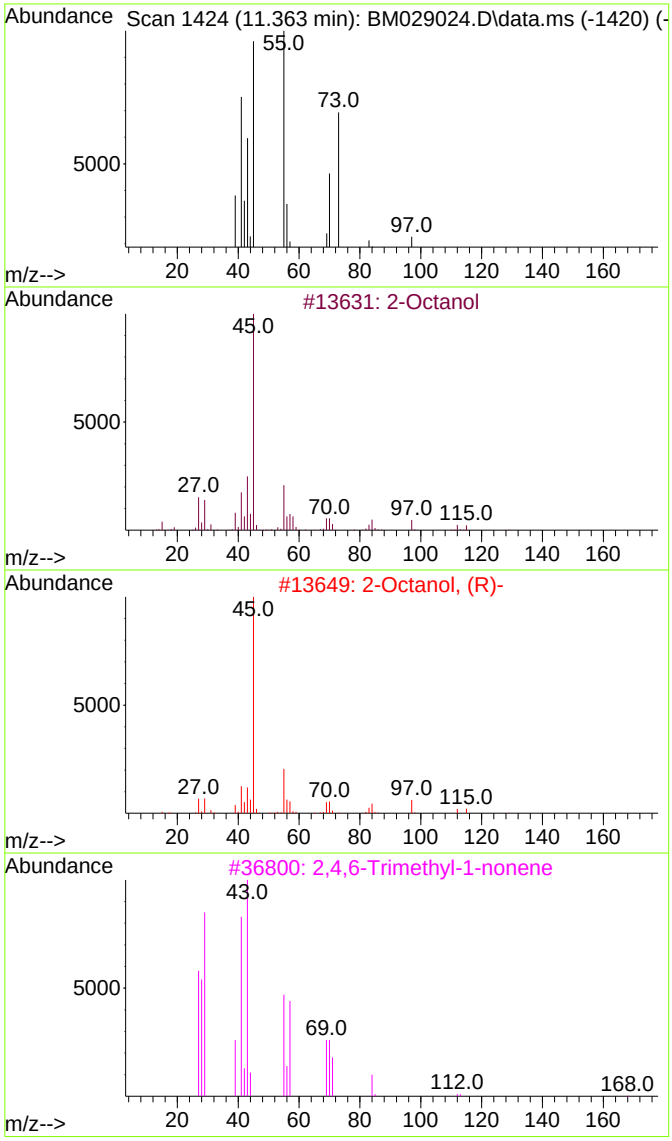
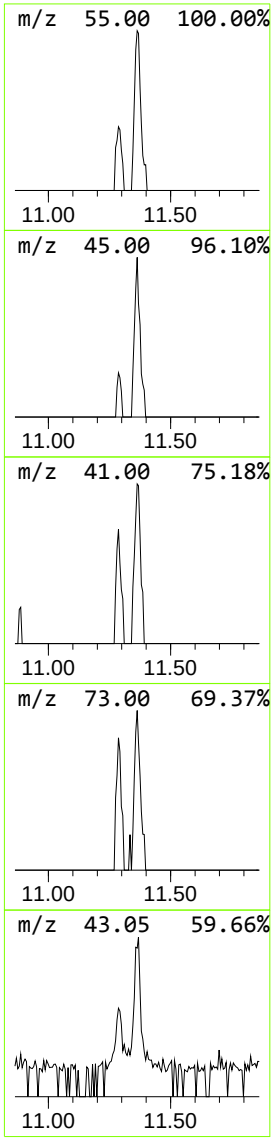
Peak Number 4 unknown11.363 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.363	3.27 ng	12144	Naphthalene-d8	10.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octanol	130	C8H18O	000123-96-6	37
2	2-Octanol, (R)-	130	C8H18O	005978-70-1	28
3	2,4,6-Trimethyl-1-nonene	168	C12H24	055771-40-9	23
4	2-Octanol, (S)-	130	C8H18O	006169-06-8	23
5	4-Pentenal, 2-ethyl-	112	C7H12O	005204-80-8	16





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Sample : M1575-05
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Instrument :
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ClientSampleId :
IDW-GW807B-AQ-030421

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

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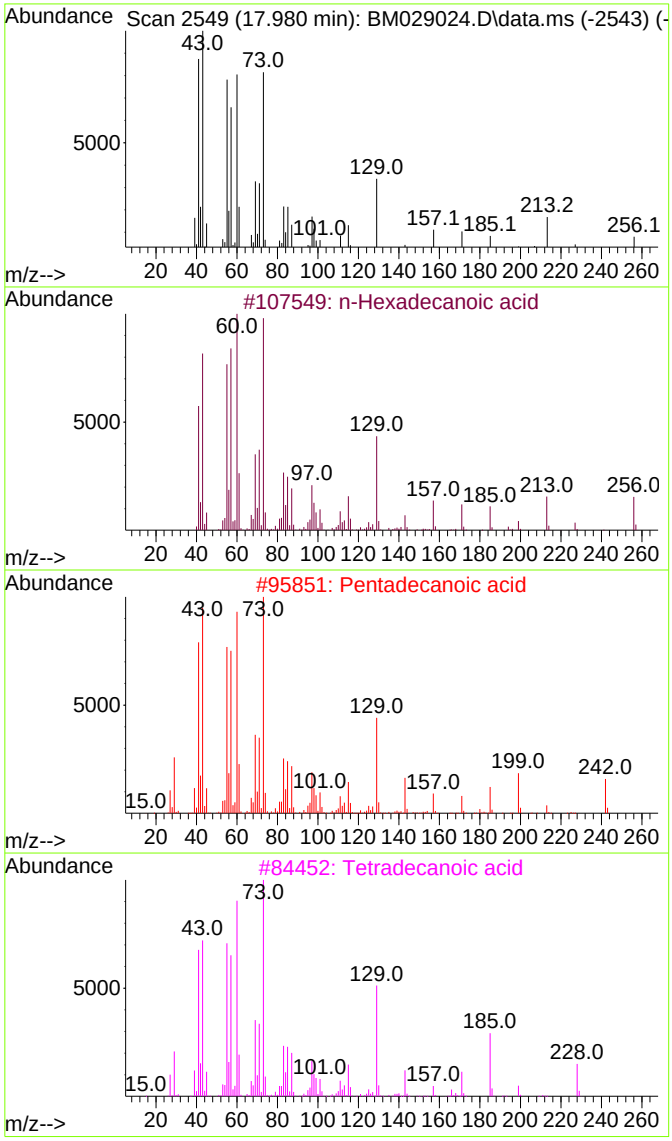
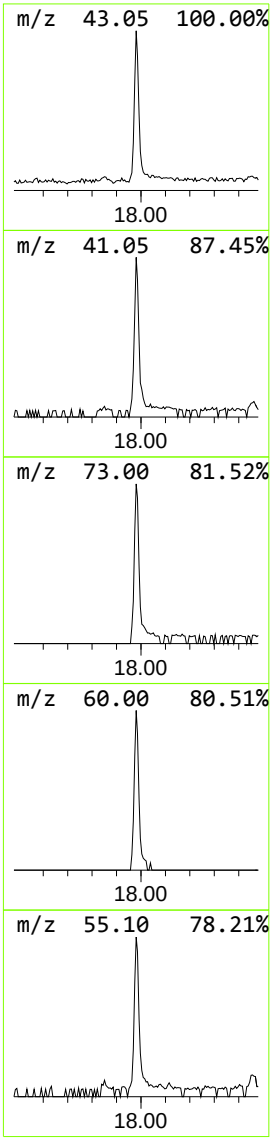
Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.980	10.72 ng	54506	Phenanthrene-d10	17.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	50





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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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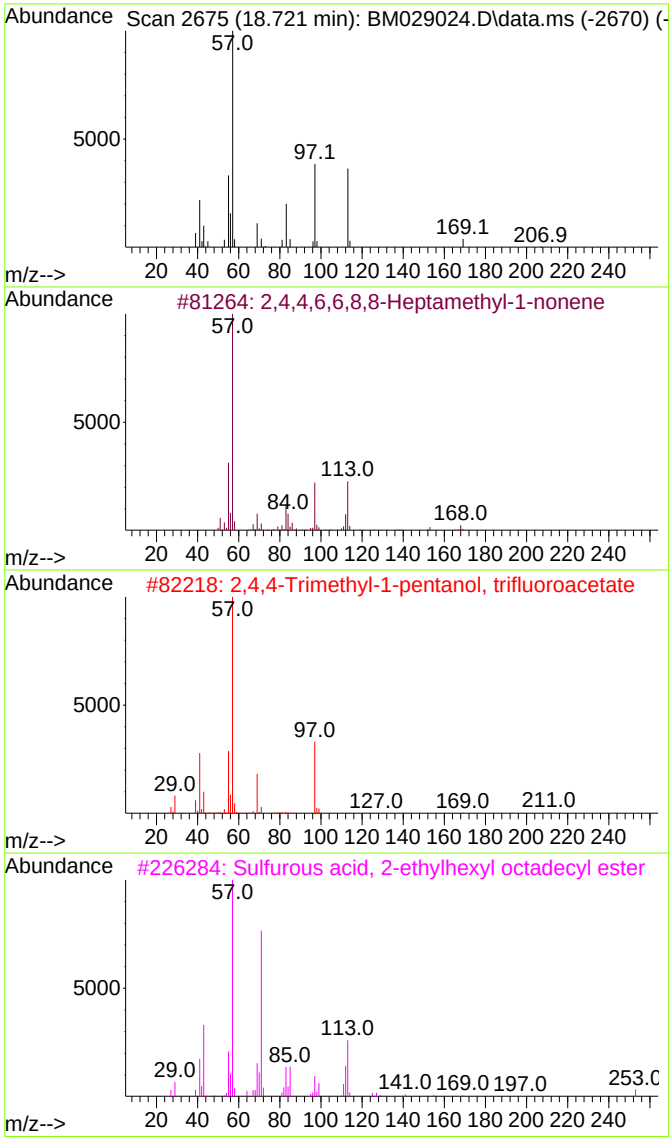
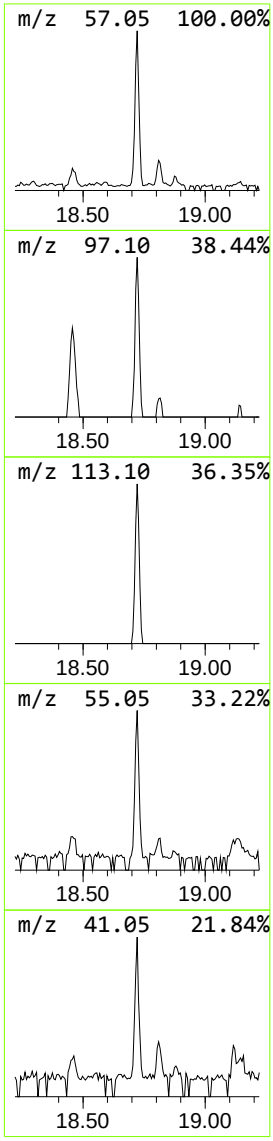
****
Peak Number 6 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.721	4.42 ng	22473	Phenanthrene-d10	17.086

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	56
2	2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2	1000365-19-5	38
3	Sulfurous acid, 2-ethylhexyl oct...	446	C26H54O3S	1000309-20-1	38
4	Octane, 2-bromo-	192	C8H17Br	000557-35-7	35
5	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	25





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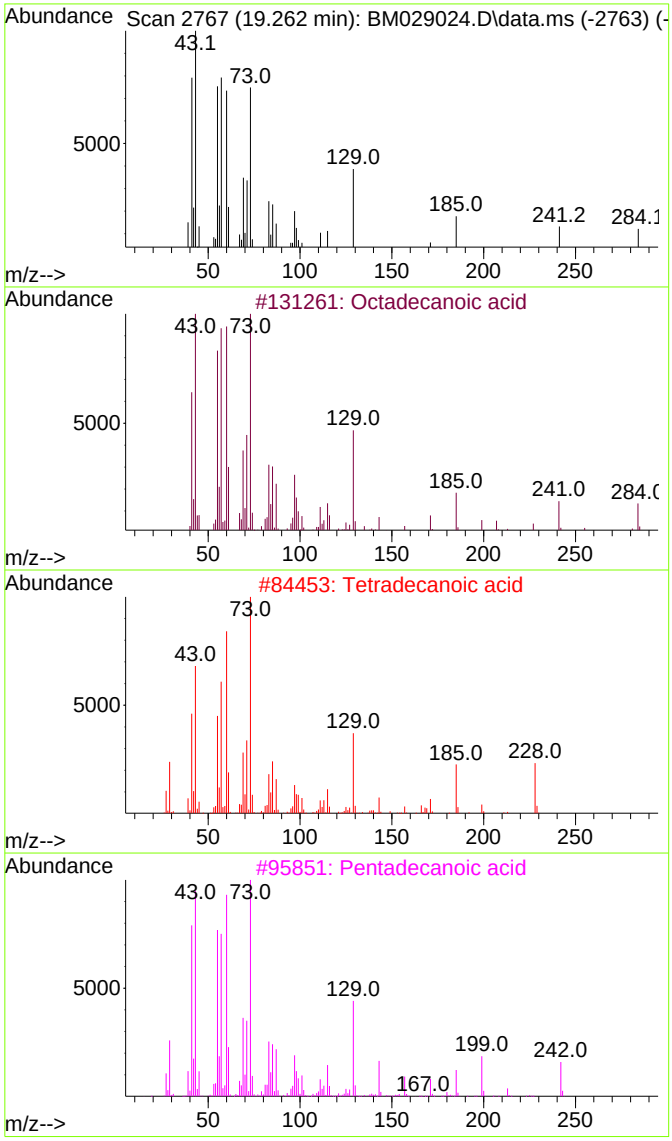
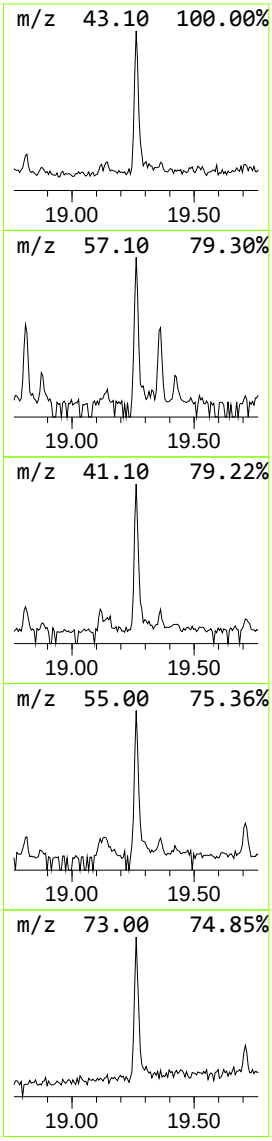
Peak Number 7 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.262	4.58 ng	29663	Chrysene-d12	21.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	58
4	n-Decanoic acid	172	C10H20O2	000334-48-5	50
5	Undecanoic acid	186	C11H22O2	000112-37-8	47





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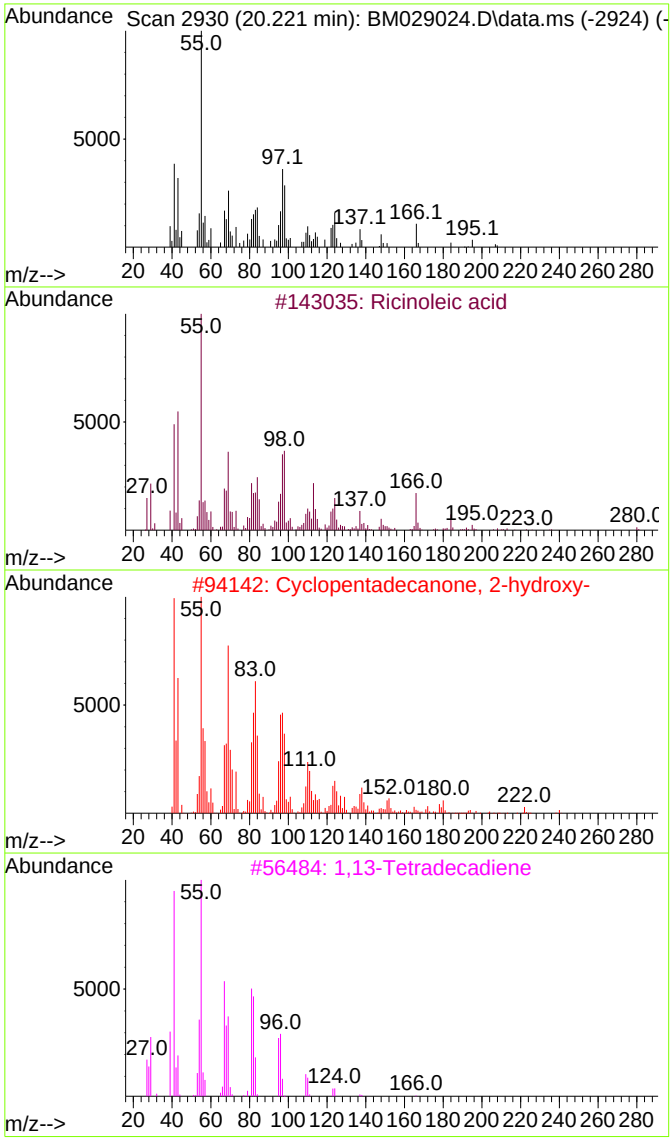
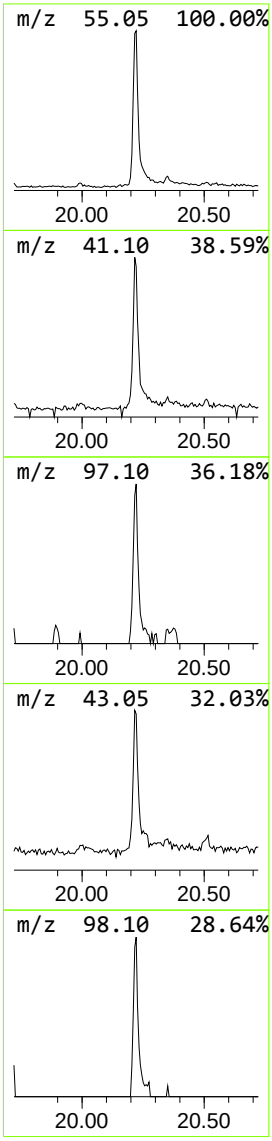
Peak Number 8 Ricinoleic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.221	12.77 ng	82739	Chrysene-d12	21.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ricinoleic acid	298	C18H34O3	000141-22-0	90
2	Cyclopentadecanone, 2-hydroxy-	240	C15H28O2	004727-18-8	49
3	1,13-Tetradecadiene	194	C14H26	021964-49-8	38
4	Dichloroacetic acid, undec-2-eny...	280	C13H22Cl2O2	1000299-43-6	30
5	1-Nonylcycloheptane	224	C16H32	1000371-47-7	27





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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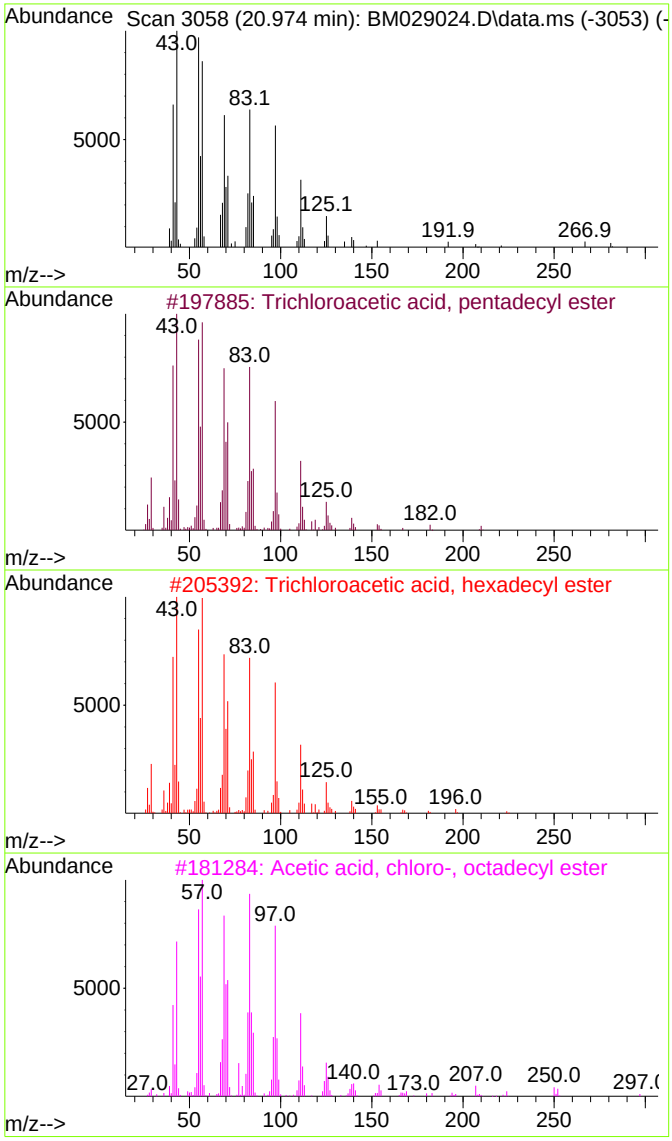
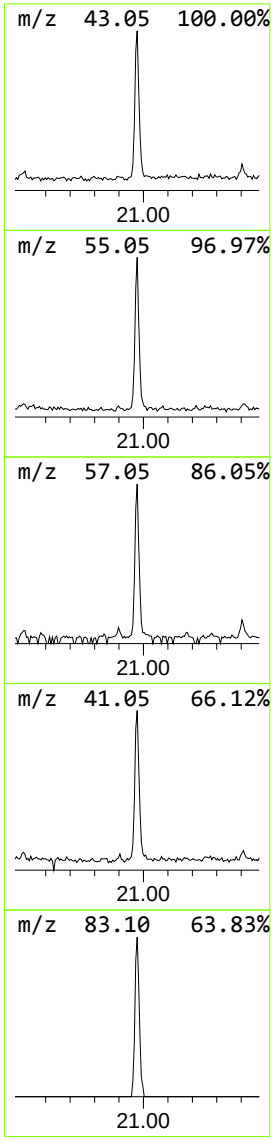
Peak Number 9 Trichloroacetic acid, penta... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.974	8.78 ng	56862	Chrysene-d12	21.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3	Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	91
4	1-Hexadecanol	242	C16H34O	036653-82-4	91
5	1,2-Octadecanediol	286	C18H38O2	020294-76-2	91





Tentatively Identified Compound (LSC) summary

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown5.722	5.722	5.9	ng	16125	1	7.669	54522	20.0
unknown8.304	8.304	2.6	ng	7118	1	7.669	54522	20.0
unknown9.887	9.887	2.8	ng	10256	2	10.463	74172	20.0
unknown11.363	11.363	3.3	ng	12144	2	10.463	74172	20.0
n-Hexadecanoic ...	17.980	10.7	ng	54506	4	17.086	101663	20.0
2,4,4,6,6,8,8-H...	18.721	4.4	ng	22473	4	17.086	101663	20.0
Octadecanoic acid	19.262	4.6	ng	29663	5	21.256	129539	20.0
Ricinoleic acid	20.221	12.8	ng	82739	5	21.256	129539	20.0
Trichloroacetic...	20.974	8.8	ng	56862	5	21.256	129539	20.0