LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011419\
Data File : BM018559.D
Acq On : 14 Jan 2019 19:47
Operator : JU/SJ
Sample : K1131-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
57-01-011019

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-BM010919.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.893	302	307	321	rVB	131692	210911	1.50%	0.293%
2	5.340	377	383	396	rBV	2725659	4241775	30.11%	5.884%
3	6.928	646	653	666	rBV	3114857	4902535	34.80%	6.800%
4	7.287	707	714	729	rBV	3209314	5024470	35.66%	6.969%
5	7.752	786	793	799	rBV	708305	1116385	7.92%	1.548%
6	8.069	840	847	855	rVB	2338797	3752030	26.63%	5.204%
7	8.916	984	991	1005	rBV	1796698	3014223	21.39%	4.181%
8	10.545	1261	1268	1276	rBV	944143	1614573	11.46%	2.239%
9	13.016	1680	1688	1701	rBV	5461801	7941695	56.37%	11.016%
10	13.857	1826	1831	1845	rBV	398500	608356	4.32%	0.844%
11	14.275	1895	1902	1915	rBV3	51840	156232	1.11%	0.217%
12	14.398	1917	1923	1937	rVB2	1516777	2399389	17.03%	3.328%
13	15.892	2167	2177	2193	rBV	4769744	6903557	49.00%	9.576%
14	17.151	2384	2391	2399	rBV	2220651	3114155	22.10%	4.319%
15	18.039	2537	2542	2553	rBV	540985	838721	5.95%	1.163%
16	19.321	2755	2760	2771	rBV2	246578	406457	2.88%	0.564%
17	19.780	2832	2838	2844	rBV	11417369	14089109	100.00%	19.542%
18	20.580	2970	2974	2977	rBV	140119	150696	1.07%	0.209%
19	21.039	3048	3052	3059	rBV	574729	693059	4.92%	0.961%
20	21.345	3098	3104	3113	rBV	3125976	4252437	30.18%	5.898%
21	21.480	3123	3127	3130	rBV	280379	289976	2.06%	0.402%
22	21.921	3198	3202	3203	rBV	339558	378236	2.68%	0.525%
23	22.392	3278	3282	3288	rVB	291931	376980	2.68%	0.523%
24	22.904	3365	3369	3374	rBV	313193	439476	3.12%	0.610%
25	23.480	3463	3467	3474	rVB2	222089	382316	2.71%	0.530%
26	23.627	3485	3492	3500	rVB	2293233	4444882	31.55%	6.165%
27	24.145	3577	3580	3588	rVB2	216447	352678	2.50%	0.489%

Sum of corrected areas: 72095309

LSC Report - Integrated Chromatogram

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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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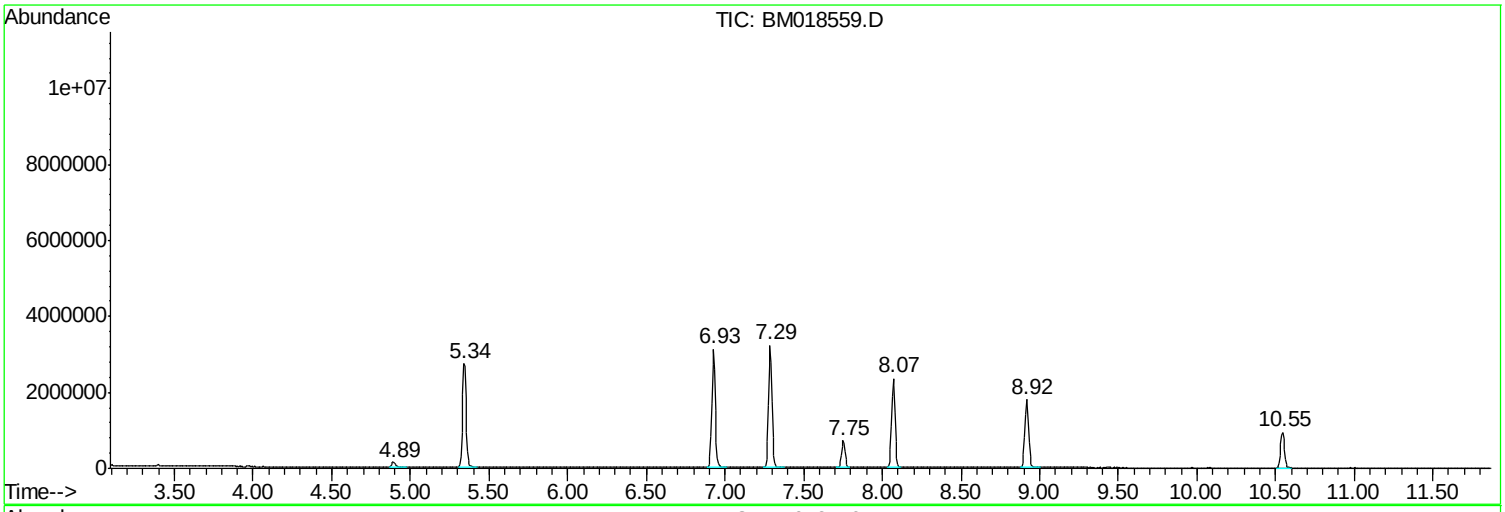
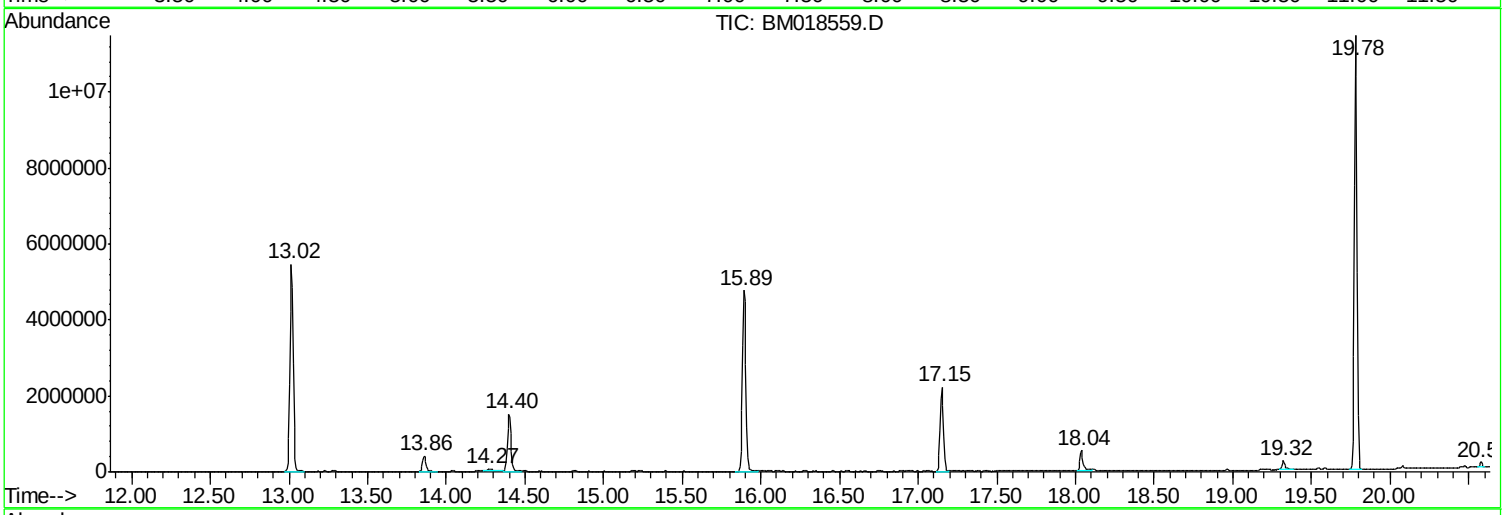
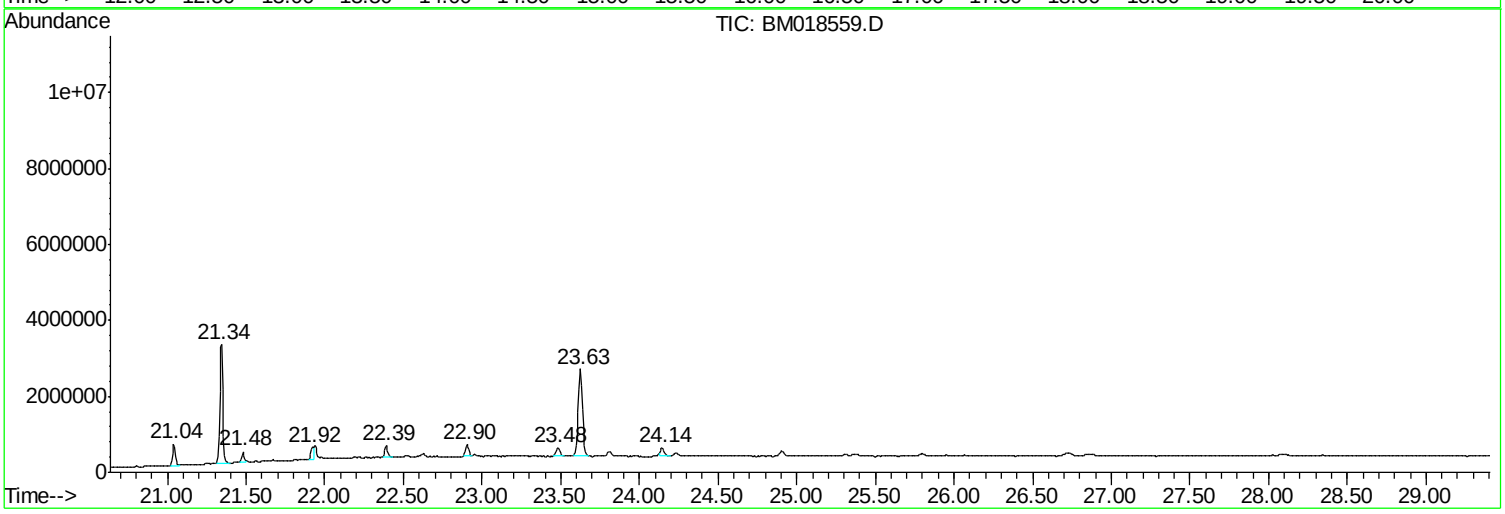
ClientSampleId :
57-01-011019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P







Library Search Compound Report

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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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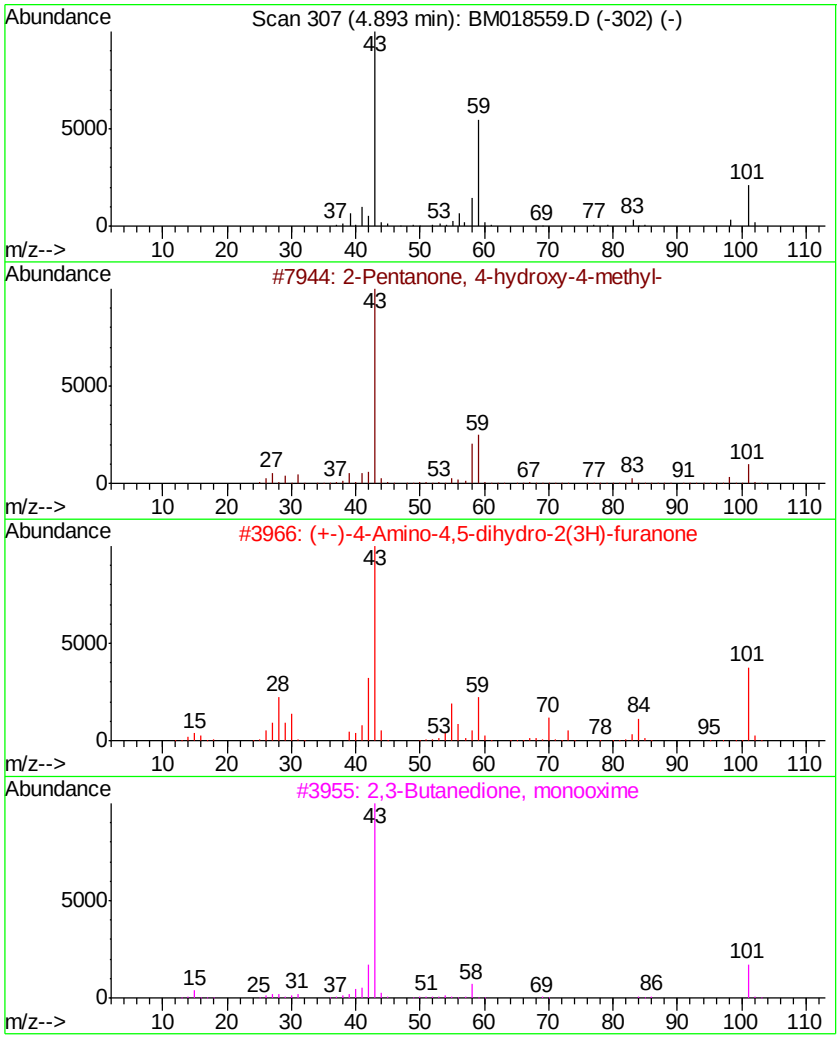
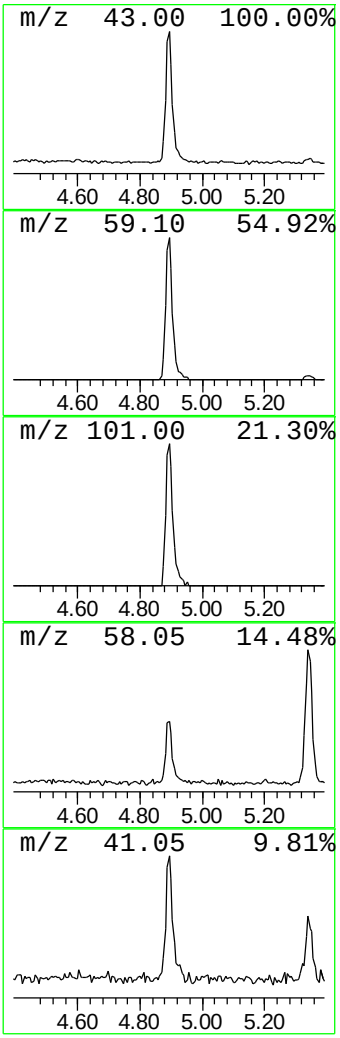
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	3.78 ng	210911	1,4-Dichlorobenzene-d4	7.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	40
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





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BNA_M
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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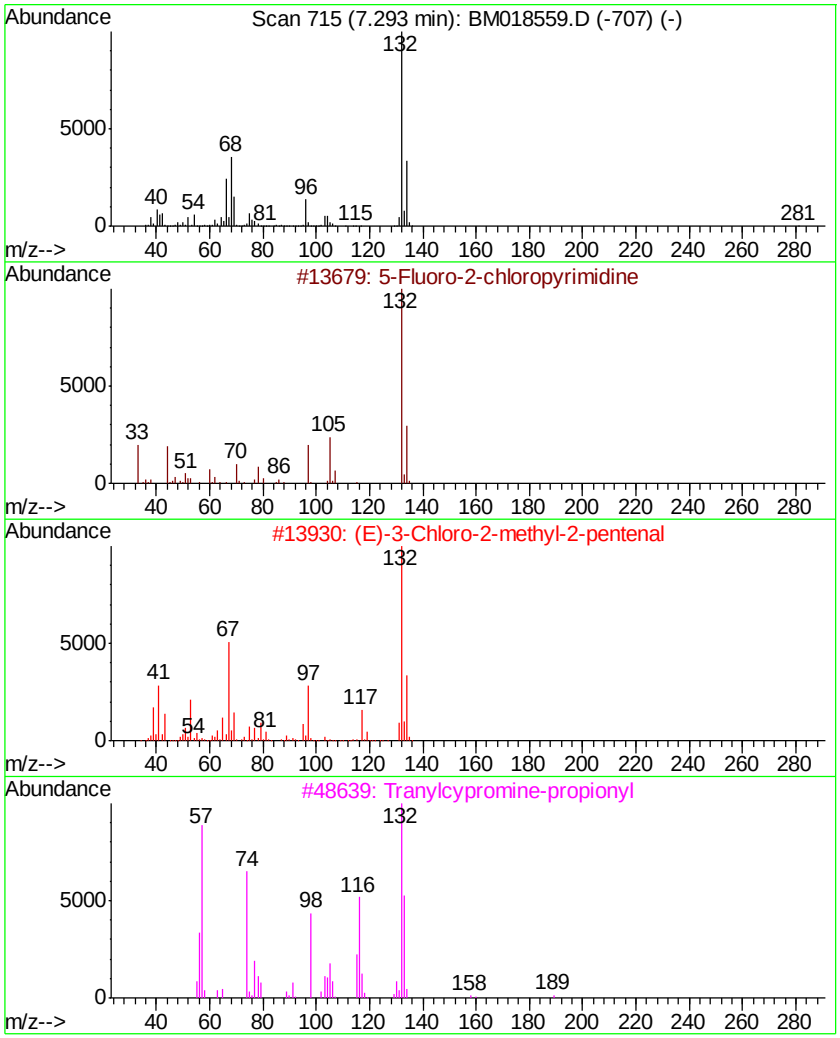
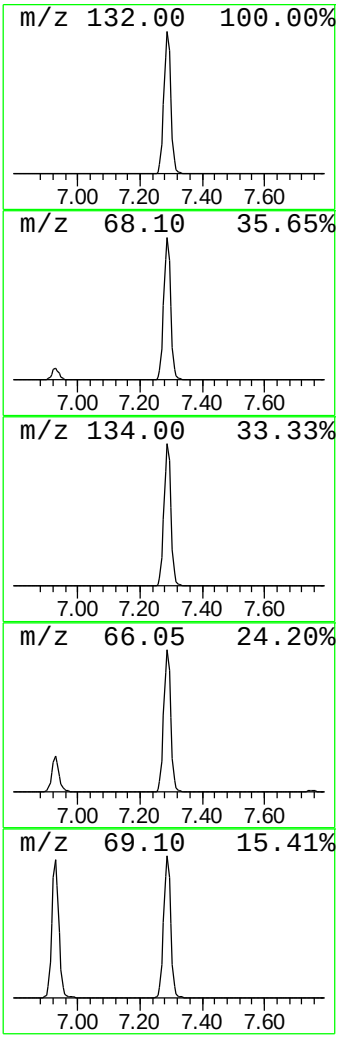
Peak Number 2 unknown7.29 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.29	90.01 ng	5024470	1,4-Dichlorobenzene-d4	7.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	25
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Instrument :
BNA_M
ClientSampleId :
57-01-011019

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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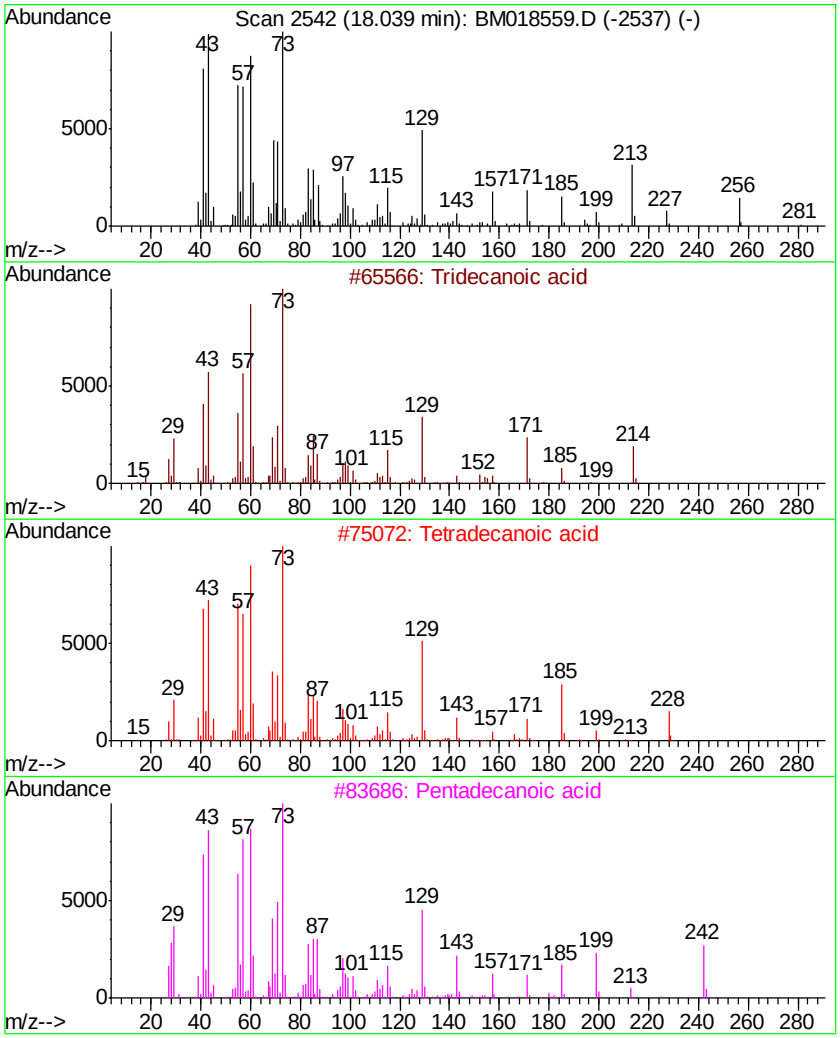
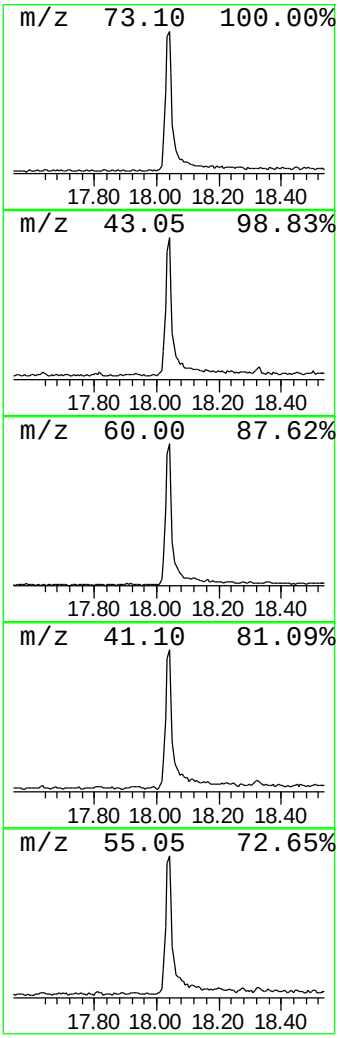
Peak Number 4 Tridecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.04	5.39 ng	838721	Phenanthrene-d10	17.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	90
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4	n-Decanoic acid	172	C10H20O2	000334-48-5	68
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58





Library Search Compound Report

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TIC Integration Parameters: LSCINT.P

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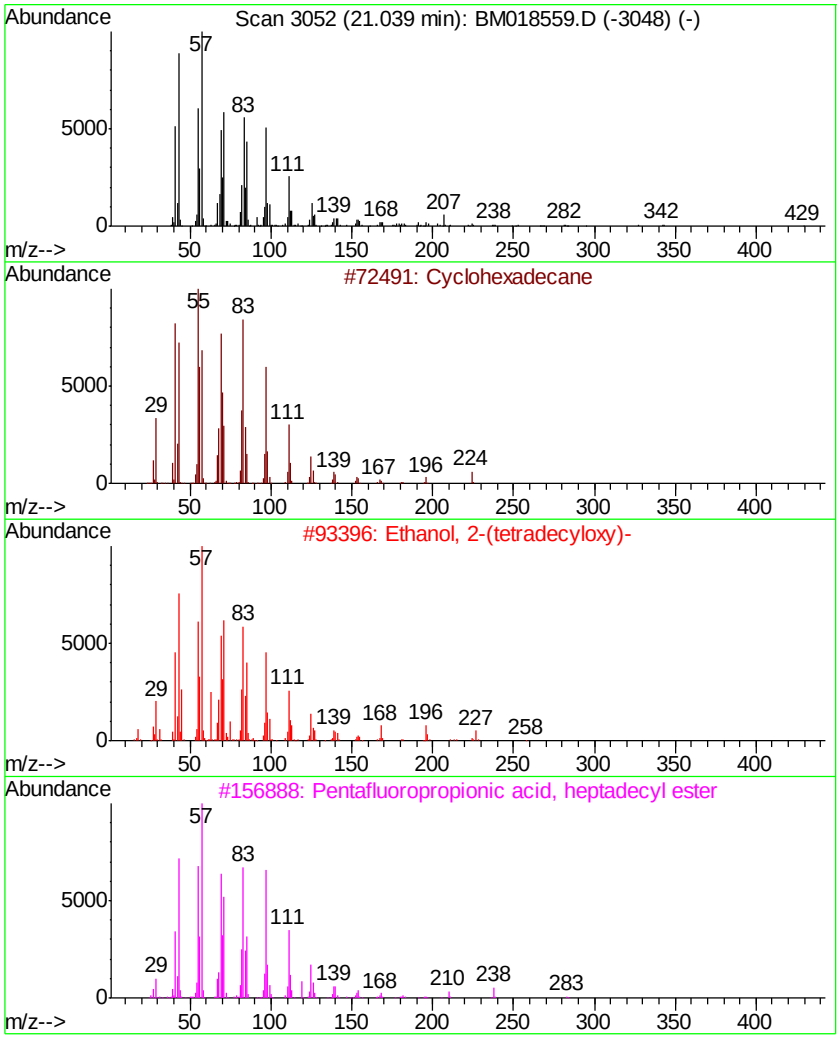
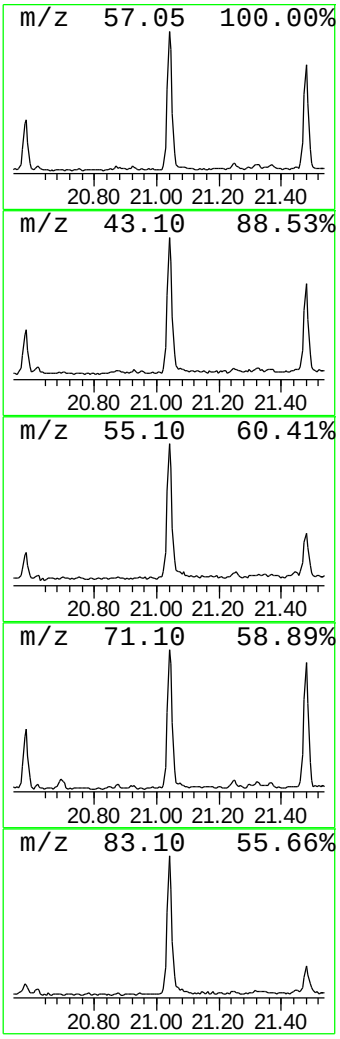
Peak Number 5 Cyclohexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.04	3.26 ng	693059	Chrysene-d12	21.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	97
2	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	90
3	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	87
4	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	87
5	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	81





Tentatively Identified Compound (LSC) summary

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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
2-Pentanone, 4-hy...	4.89	3.8	ng	210911	1	7.75	1116390	20.0
unknown7.29	7.29	90.0	ng	5024470	1	7.75	1116390	20.0
Tridecanoic acid	18.04	5.4	ng	838721	4	17.15	3114160	20.0
Cyclohexadecane	21.04	3.3	ng	693059	5	21.34	4252440	20.0