LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120820\
Data File : BF122588.D
Acq On : 8 Dec 2020 15:07
Operator : JU/CG
Sample : L4970-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 4S2-A-D-COMP

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_F\METHODS\8270-BF120520.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122588.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.422	392	397	404	rBV	463581	536555	14.50%	1.707%
2	5.046	498	503	510	rBV	571282	698643	18.88%	2.222%
3	5.457	568	573	576	rBV	3026949	2821776	76.25%	8.976%
4	5.851	637	640	646	rBB	91095	74627	2.02%	0.237%
5	6.469	740	745	761	rBV	3067957	3057666	82.62%	9.727%
6	6.840	804	808	811	rBV	1058108	913968	24.70%	2.907%
7	7.398	898	903	906	rBV	2150700	1874982	50.66%	5.965%
8	8.122	1022	1026	1029	rBV	1511509	1216004	32.86%	3.868%
9	9.198	1204	1209	1212	rBV	3902749	3303990	89.28%	10.510%
10	9.592	1272	1276	1280	rBV	306340	300120	8.11%	0.955%
11	9.745	1299	1302	1304	rBV3	52552	55422	1.50%	0.176%
12	9.792	1307	1310	1312	rVB	56390	51109	1.38%	0.163%
13	9.875	1318	1324	1328	rBV	1664787	1522371	41.14%	4.843%
14	10.286	1391	1394	1399	rBV3	87861	85538	2.31%	0.272%
15	10.663	1454	1458	1463	rBV	2357998	2306635	62.33%	7.338%
16	11.363	1574	1577	1581	rBV	1821893	1481145	40.02%	4.712%
17	11.904	1665	1669	1676	rBV	1494632	1635057	44.18%	5.201%
18	12.698	1799	1804	1812	rVB	3056180	3700883	100.00%	11.773%
19	12.951	1843	1847	1851	rBV	3354469	3201044	86.49%	10.183%
20	14.004	2023	2026	2033	rVB	1422865	1361258	36.78%	4.330%
21	15.468	2270	2275	2286	rVB	872306	1236858	33.42%	3.935%

Sum of corrected areas: 31435651

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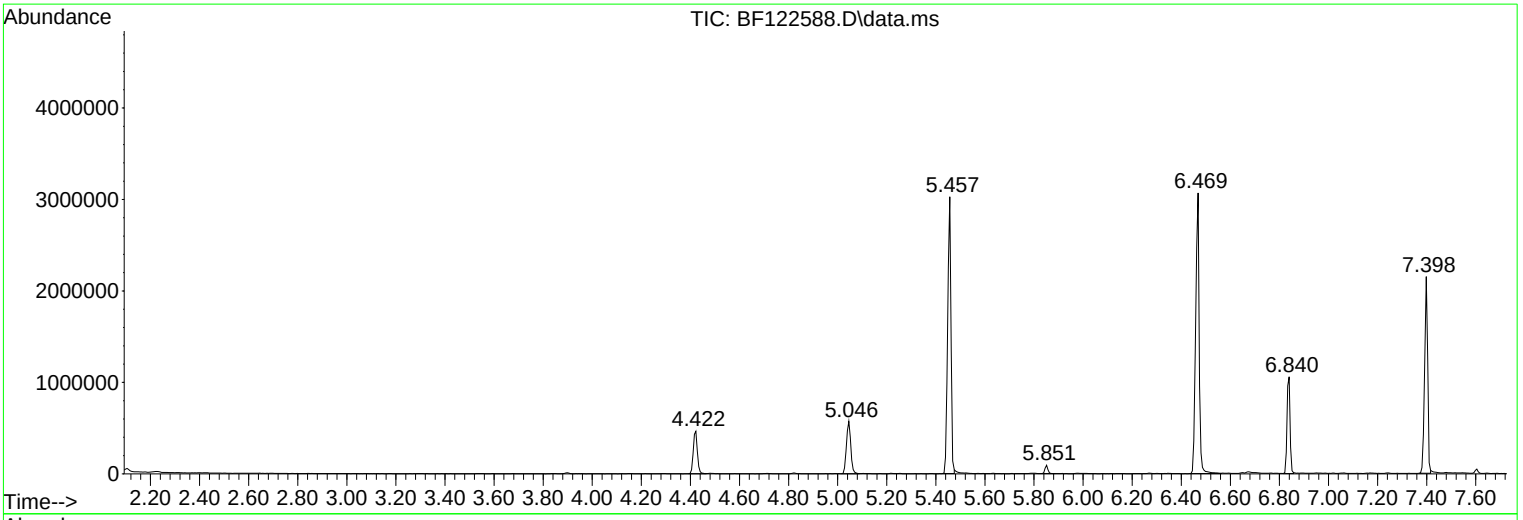
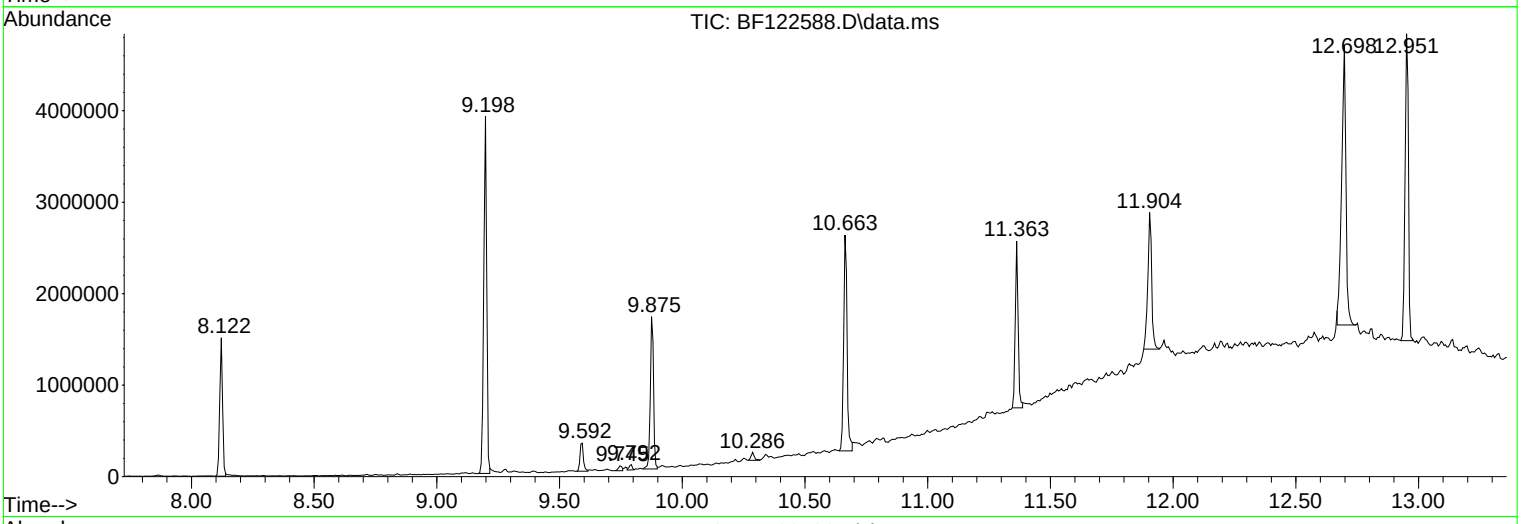
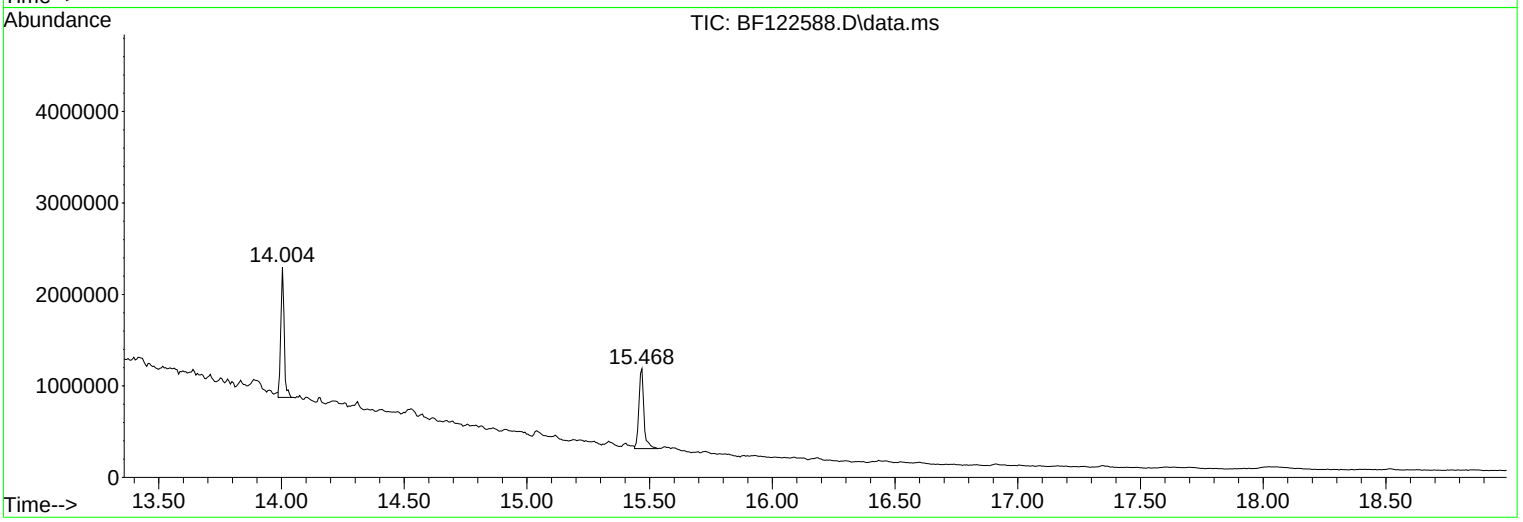
Instrument :
BNA_F
ClientSampleId :
4S2-A-D-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.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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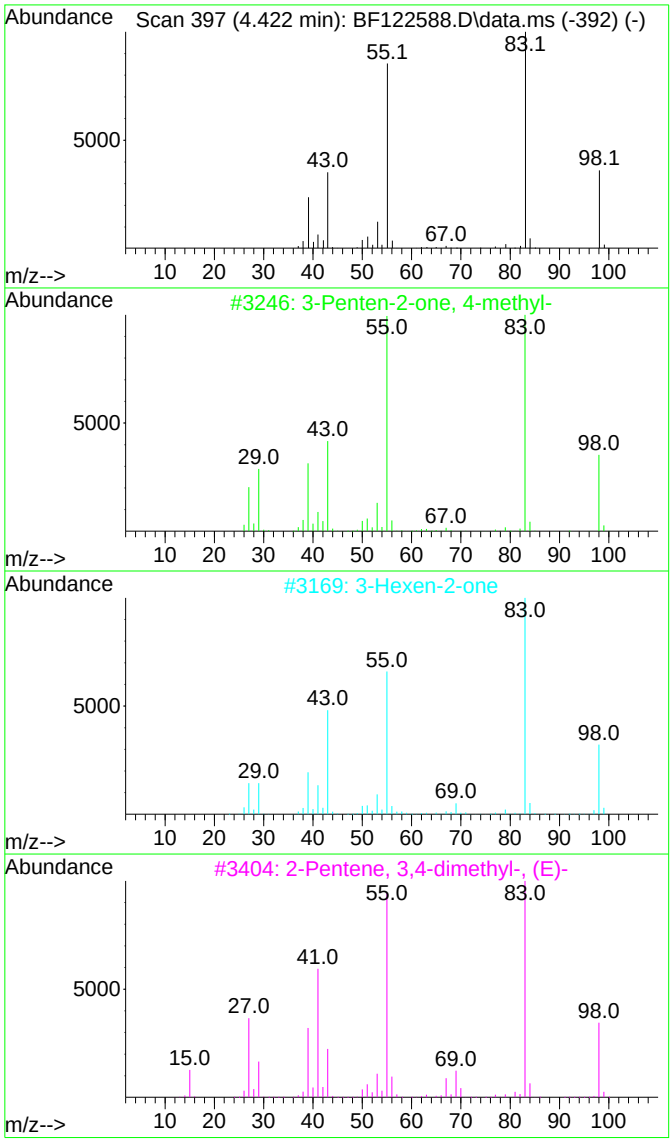
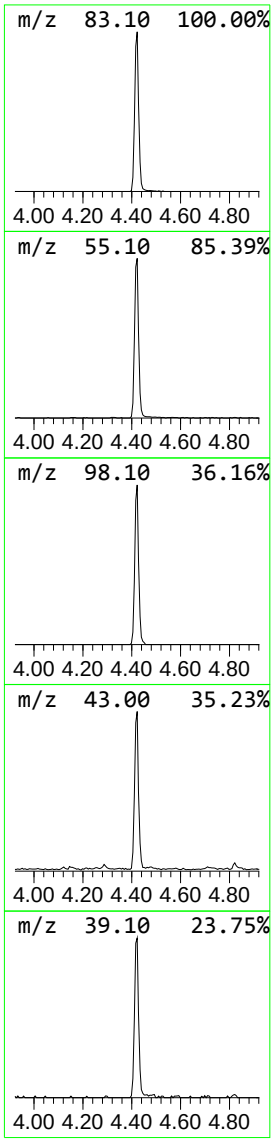
Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.422	11.74 ng	536555	1,4-Dichlorobenzene-d4	6.840

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	90
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80





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Instrument : BNA_F
ClientSampleId : 4S2-A-D-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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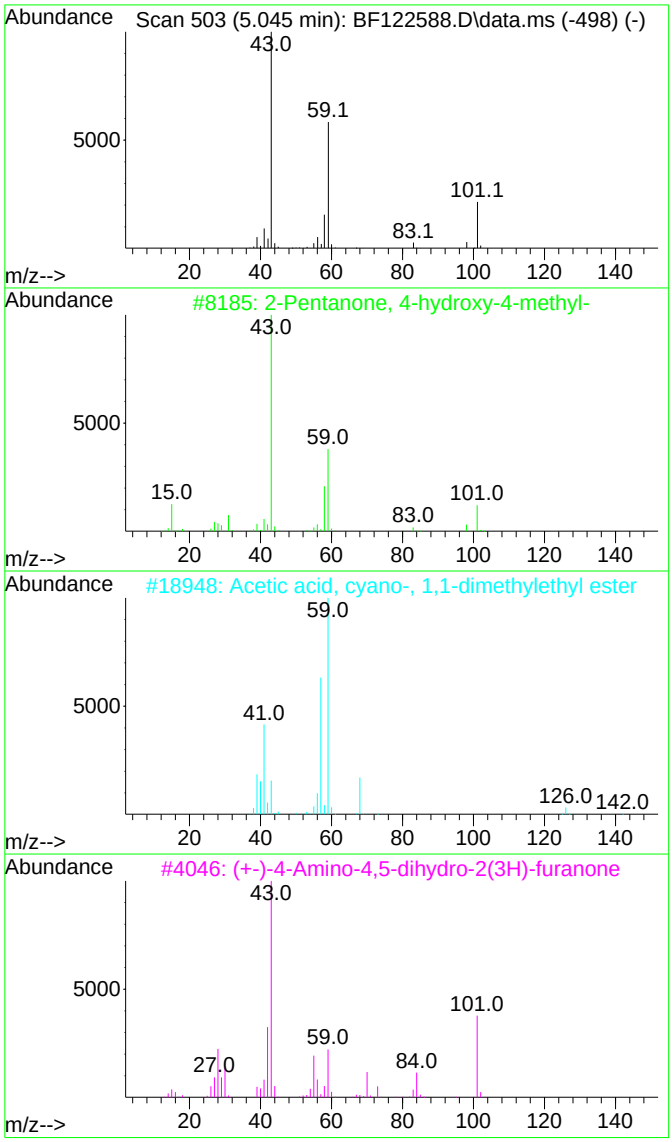
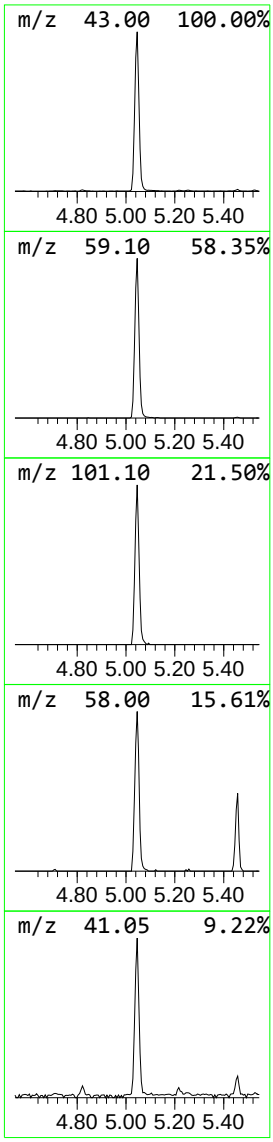
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.045	15.29 ng	698643	1,4-Dichlorobenzene-d4	6.840

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	25
3	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Sample : L4970-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
4S2-A-D-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.M
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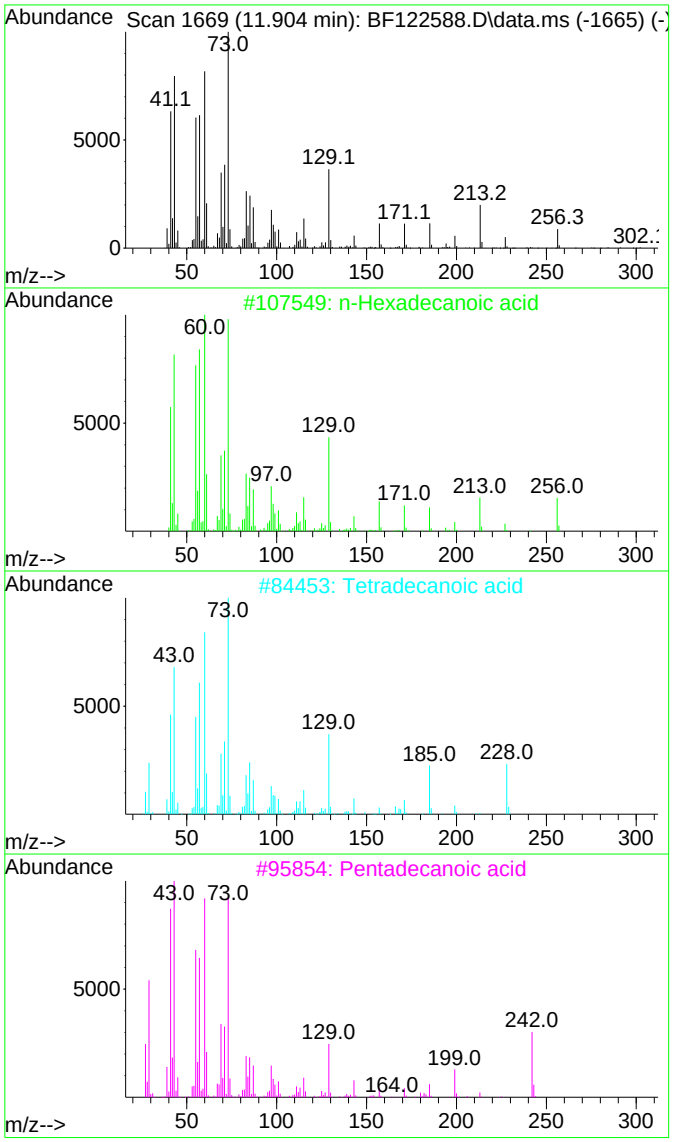
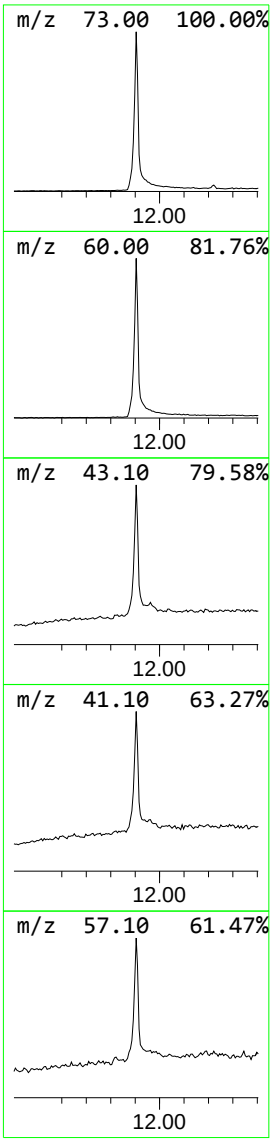
Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.904	22.08 ng	1635060	Phenanthrene-d10	11.363

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Octadecanoic acid	284	C18H36O2	000057-11-4	81
5	Tridecanoic acid	214	C13H26O2	000638-53-9	70





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Instrument :
BNA_F
ClientSampleId :
4S2-A-D-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.M
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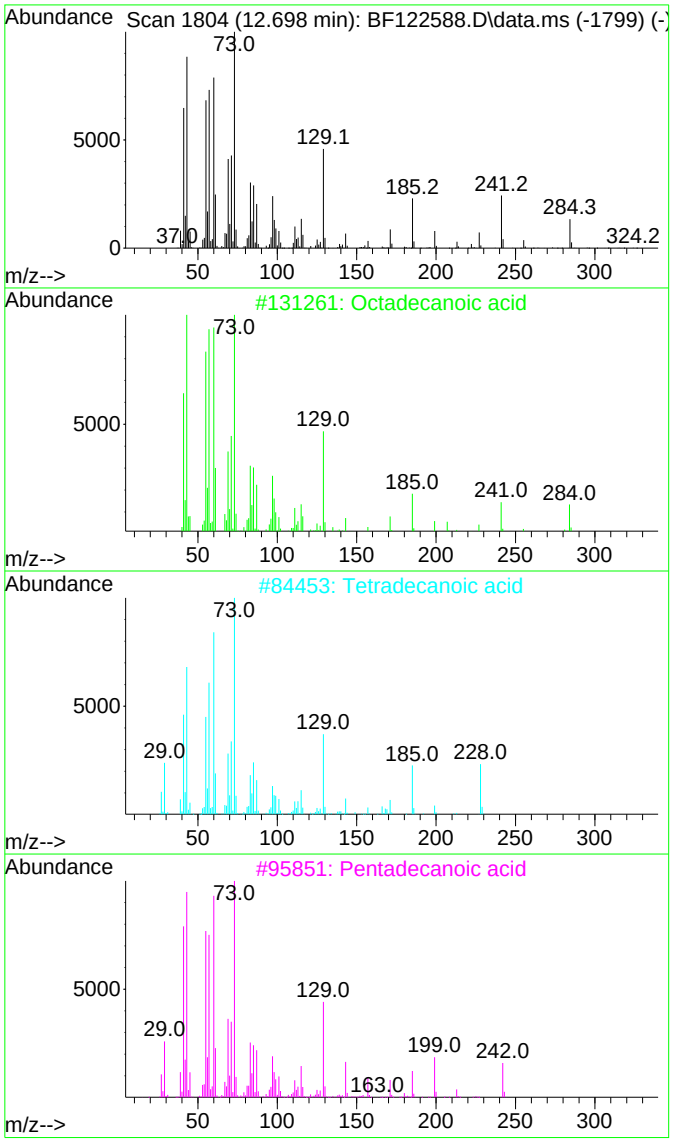
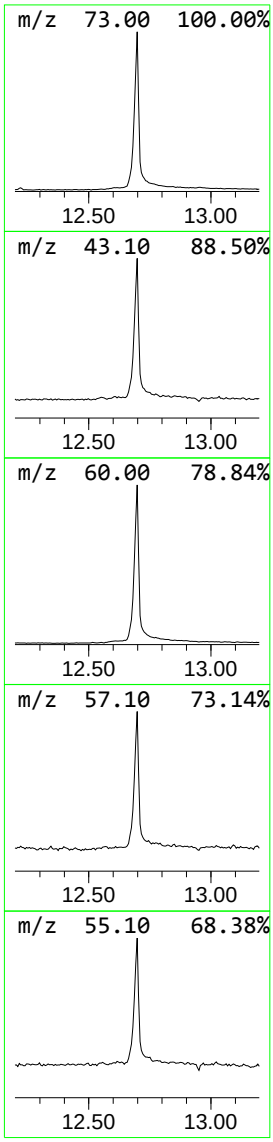
****
Peak Number 4 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.698	54.37 ng	3700880	Chrysene-d12	14.004

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	87
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	Tridecanoic acid	214	C13H26O2	000638-53-9	68
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-one,...	4.422	11.7	ng	536555	1	6.840	913968	20.0
2-Pentanone, 4-...	5.045	15.3	ng	698643	1	6.840	913968	20.0
n-Hexadecanoic ...	11.904	22.1	ng	1635060	4	11.363	1481150	20.0
Octadecanoic acid	12.698	54.4	ng	3700880	5	14.004	1361260	20.0