LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082124\
Data File : BP021604.D
Acq On : 21 Aug 2024 19:35
Operator : RC/JU
Sample : P3617-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
VCPS-B2-081424-6W-DUP

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_P\Methods\8270E-BP081324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP021604.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.028	3	7	26	rVB	9394597	11835459	77.50%	17.877%
2	4.940	326	332	340	rVB2	103039	161528	1.06%	0.244%
3	5.393	402	409	421	rBV	1737421	2654380	17.38%	4.009%
4	6.963	669	676	686	rBV	1087574	1691172	11.07%	2.554%
5	7.799	810	818	825	rBV	677720	1110290	7.27%	1.677%
6	8.946	1005	1013	1025	rBV	2085839	3631755	23.78%	5.486%
7	10.587	1282	1292	1304	rBV	849047	1494114	9.78%	2.257%
8	11.334	1411	1419	1431	rBV	84886	196237	1.28%	0.296%
9	11.504	1441	1448	1458	rBV	81990	183324	1.20%	0.277%
10	13.057	1704	1712	1726	rBV	4764206	7435042	48.68%	11.230%
11	14.445	1937	1948	1957	rBV	1280070	2005677	13.13%	3.029%
12	15.963	2198	2206	2230	rBV	4699678	7289285	47.73%	11.010%
13	17.257	2419	2426	2434	rBV	1818477	2593229	16.98%	3.917%
14	18.198	2581	2586	2596	rBV	161616	264933	1.73%	0.400%
15	19.674	2833	2837	2844	rBV	925343	1125794	7.37%	1.700%
16	19.980	2883	2889	2899	rBV	11994567	15271892	100.00%	23.068%
17	21.386	3125	3128	3135	rVB	186701	257669	1.69%	0.389%
18	21.716	3178	3184	3197	rBV2	2190400	3339288	21.87%	5.044%
19	25.151	3759	3768	3779	rVB	1371993	3664089	23.99%	5.534%

Sum of corrected areas: 66205157

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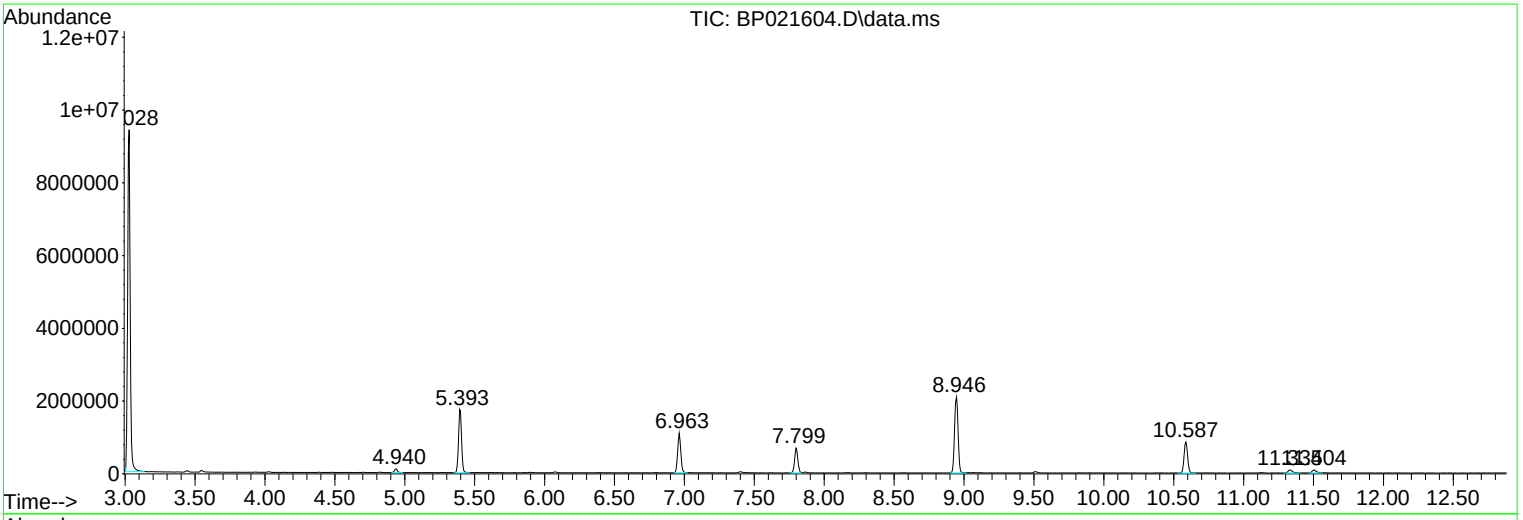
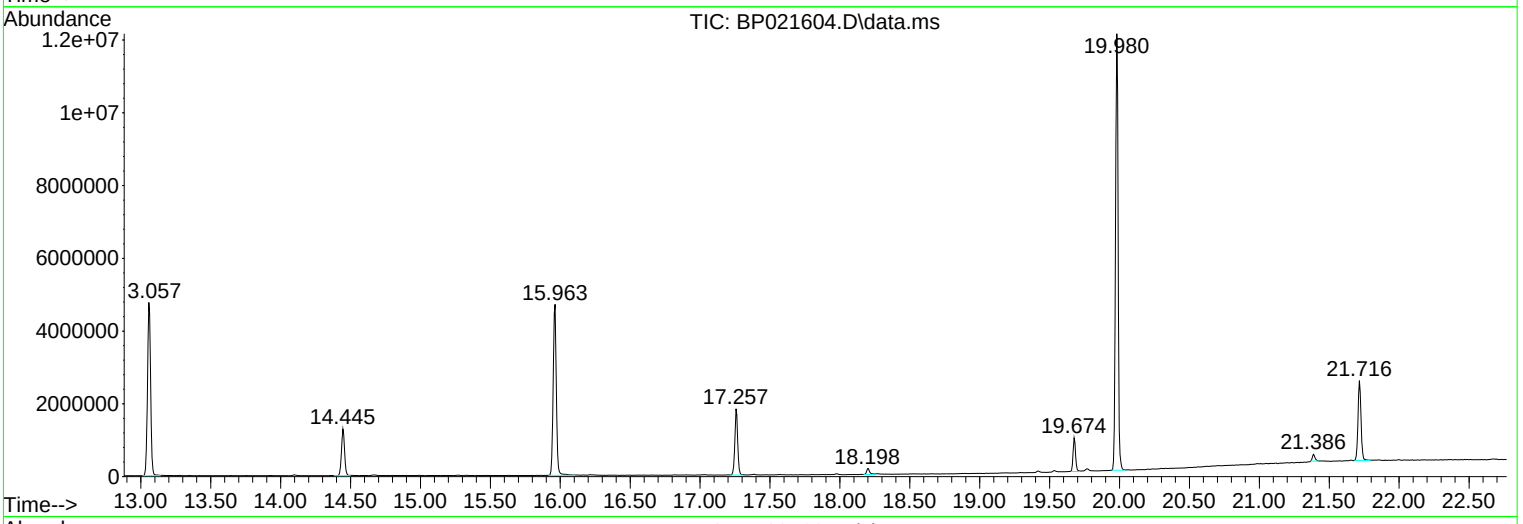
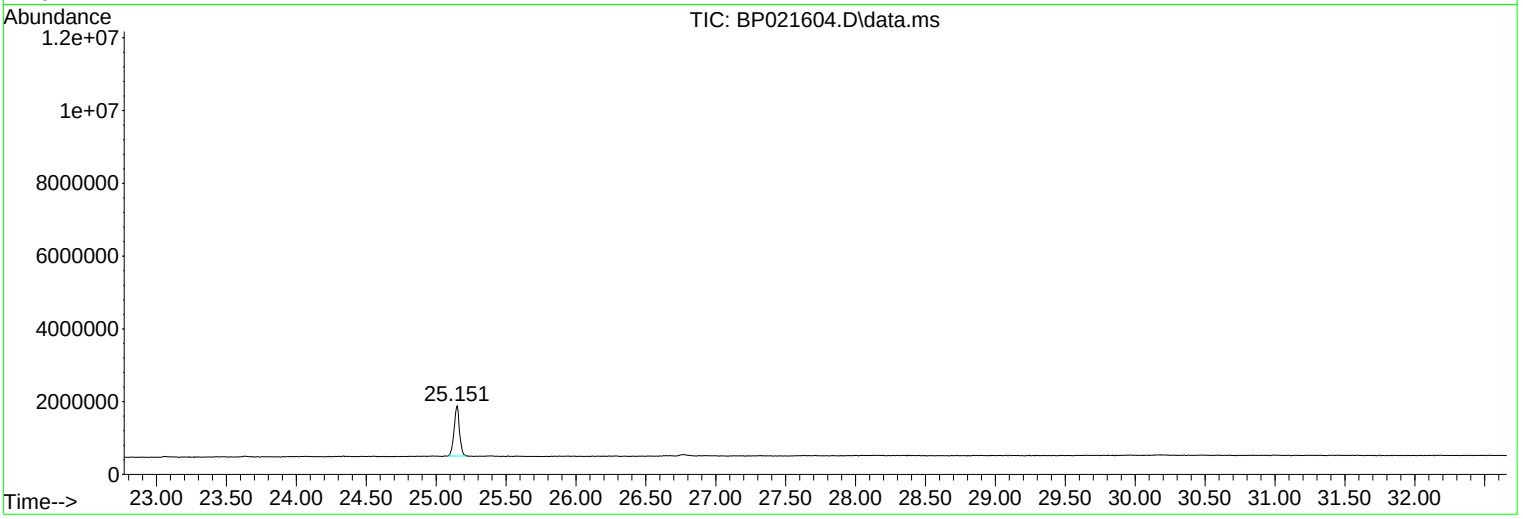
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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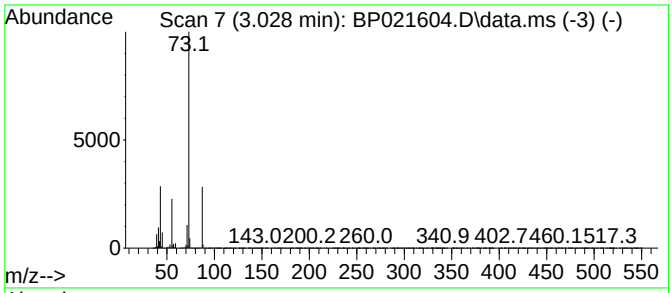
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

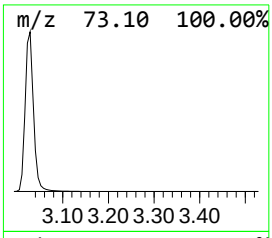
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

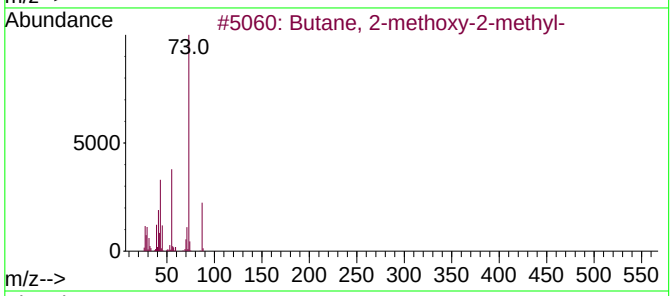
****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

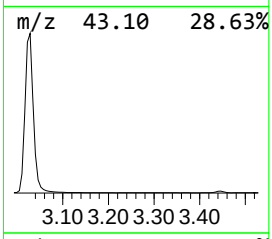
R.T.	EstConc	Area	Relative to ISTD	R.T.
3.028	213.20 ng	11835500	1,4-Dichlorobenzene-d4	7.799

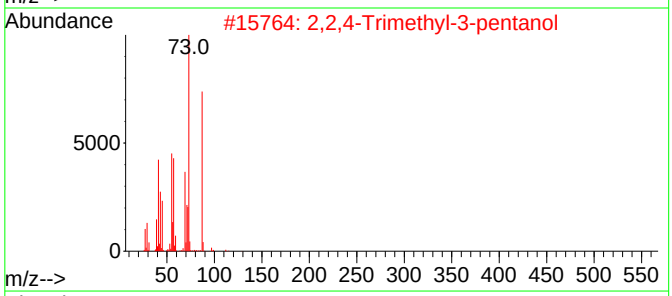
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9

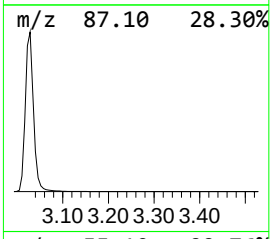


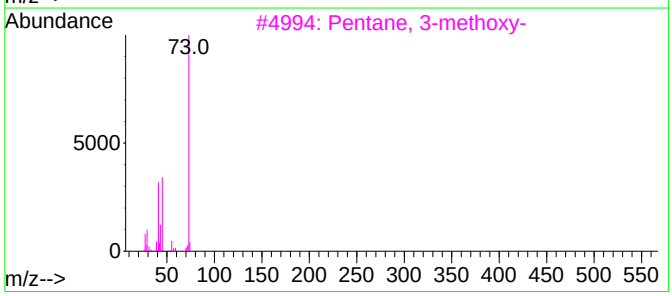


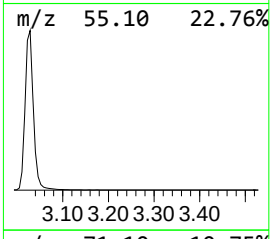


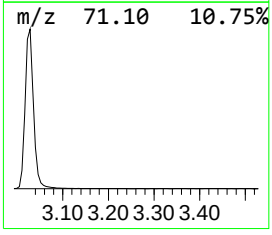












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Instrument :
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ClientSampleId :
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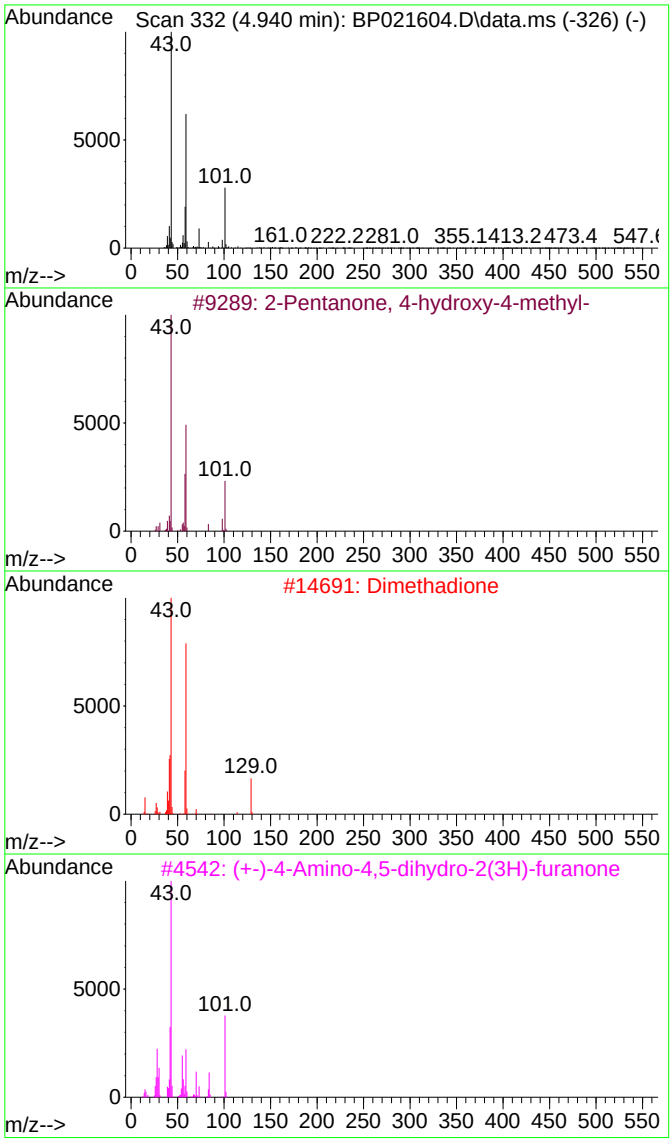
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

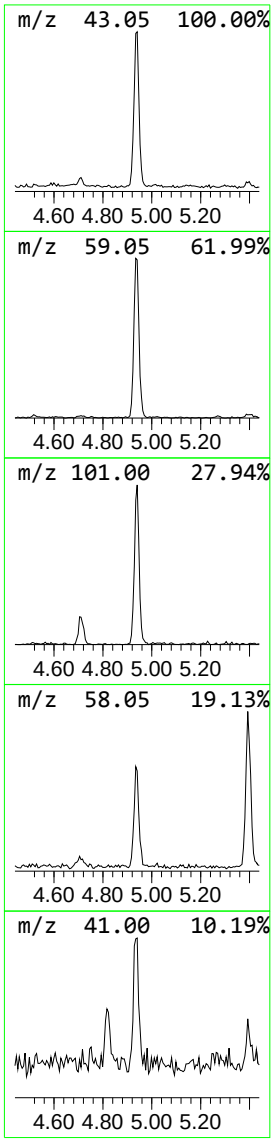
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.940	2.91 ng	161528	1,4-Dichlorobenzene-d4	7.799

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2	Dimethadione	129	C5H7NO3	000695-53-4	40
3	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	37
4	(2,3,3-Trimethyloxiranyl)methanol	116	C6H12O2	1000306-64-7	36
5	Methyl 2,5,8,11-tetraoxatridecan...	236	C10H20O6	1000366-78-2	28





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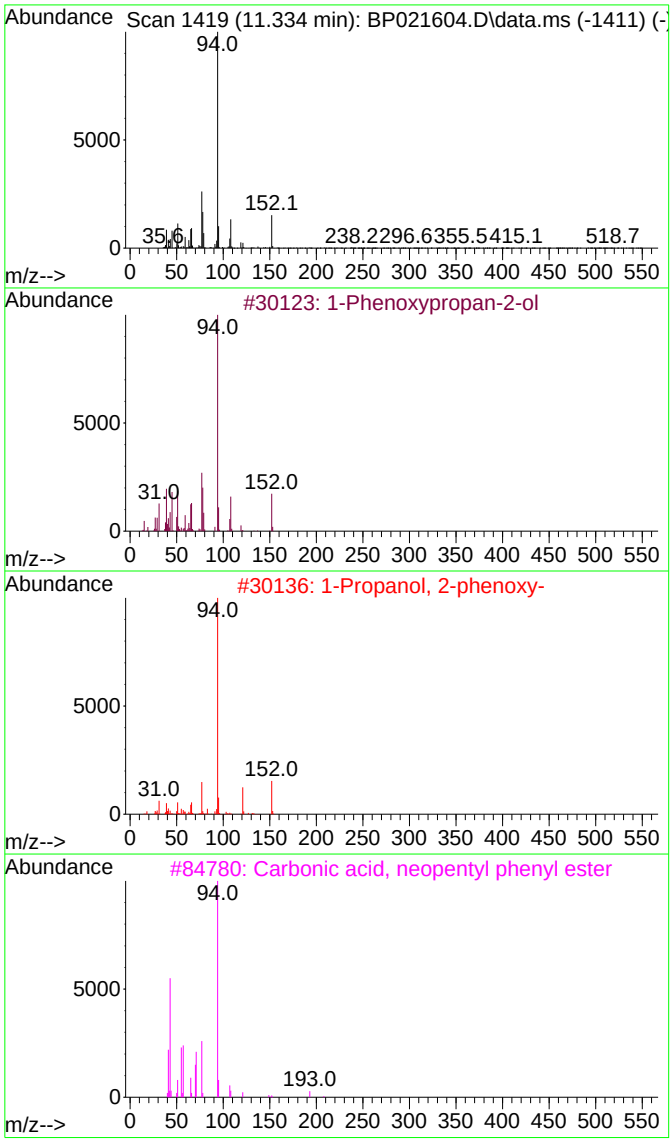
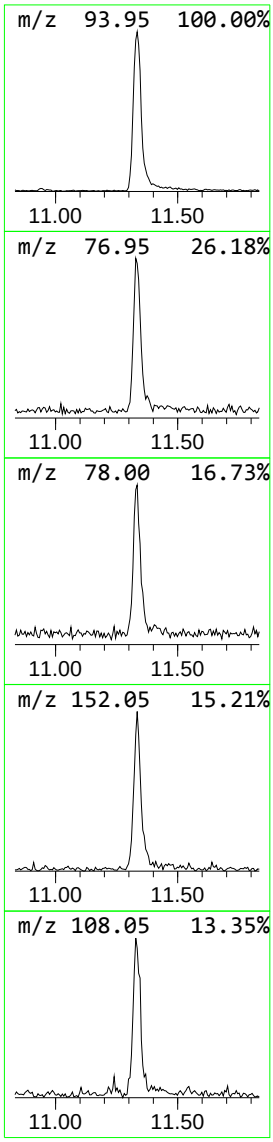
****

Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.334	2.63 ng	196237	Naphthalene-d8	10.587

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	94
2	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
3	Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59
4	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	58
5	Benzene, (1-methylpropoxy)-	150	C10H14O	010574-17-1	53





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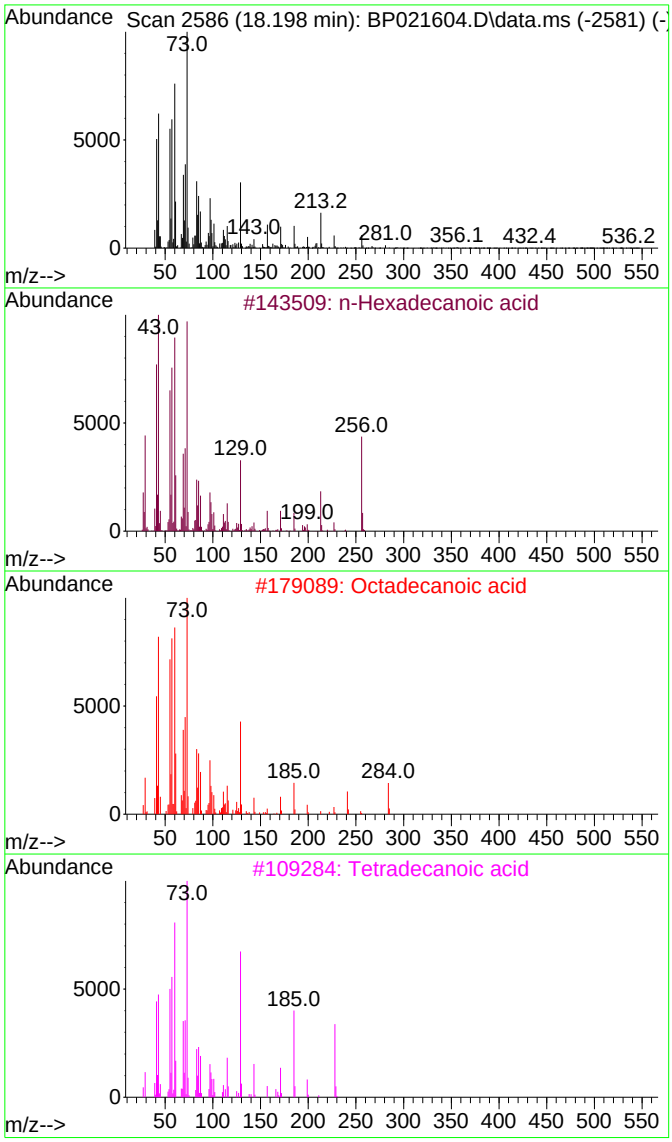
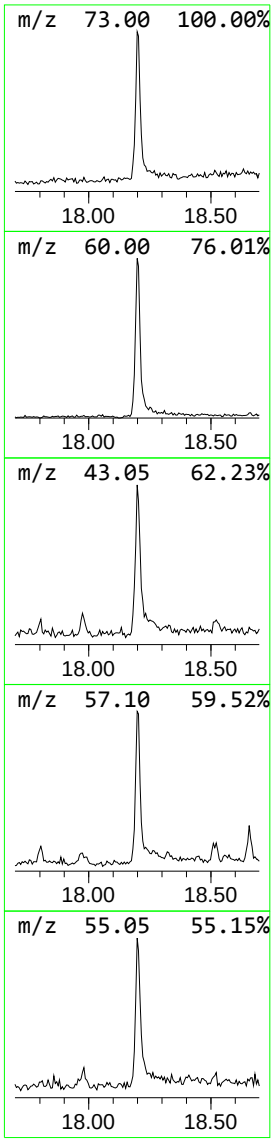
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.198	2.04 ng	264933	Phenanthrene-d10	17.257

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Octadecanoic acid	284	C18H36O2	000057-11-4	80
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5	Dodecanoic acid	200	C12H24O2	000143-07-7	58





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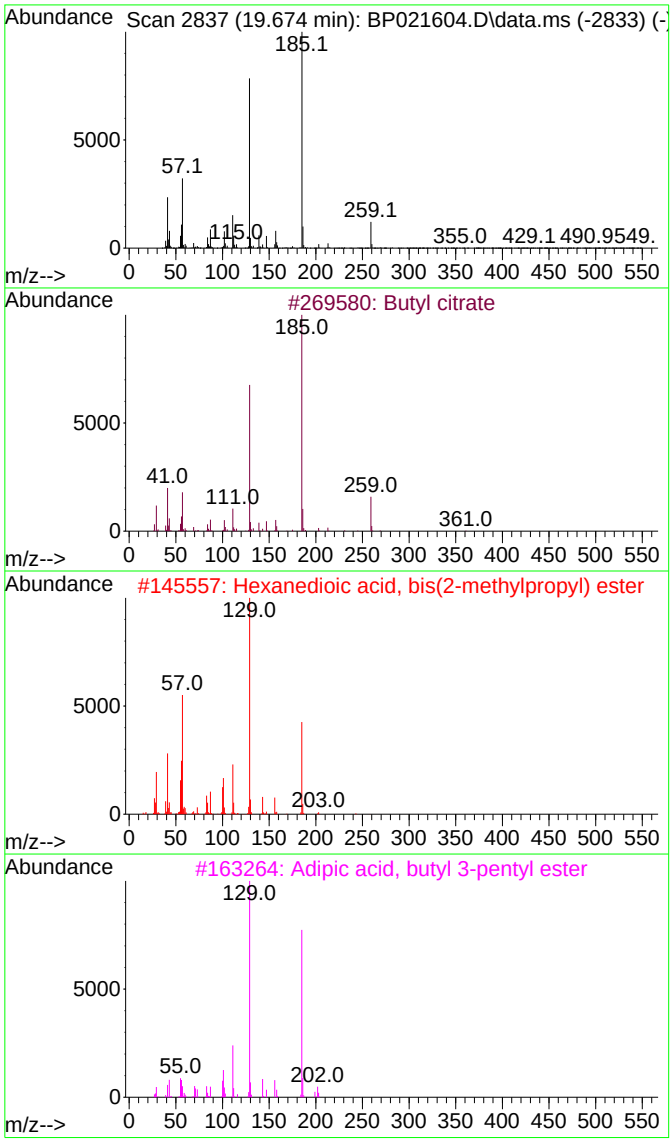
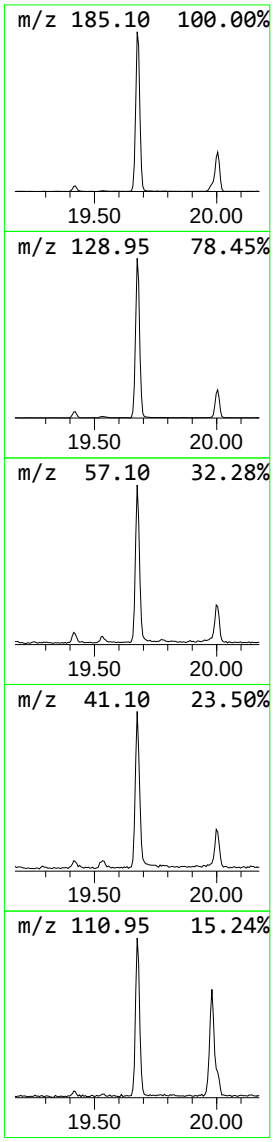
****

Peak Number 5 Butyl citrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.674	6.74 ng	1125790	Chrysene-d12	21.716

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl citrate	360	C18H32O7	000077-94-1	81
2	Hexanedioic acid, bis(2-methylpr...	258	C14H26O4	000141-04-8	72
3	Adipic acid, butyl 3-pentyl ester	272	C15H28O4	1000324-60-5	72
4	Adipic acid, 3-hexyl isobutyl ester	286	C16H30O4	1000353-62-2	56
5	Adipic acid, 2-decyl isobutyl ester	342	C20H38O4	1000353-59-6	56





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	3.028	213.2	ng	11835500	1	7.799	1110290	20.0
2-Pentanone, 4-...	4.940	2.9	ng	161528	1	7.799	1110290	20.0
1-Phenoxypropan...	11.334	2.6	ng	196237	2	10.587	1494110	20.0
n-Hexadecanoic ...	18.198	2.0	ng	264933	4	17.257	2593230	20.0
Butyl citrate	19.674	6.7	ng	1125790	5	21.716	3339290	20.0