LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP012723\
Data File : BP013616.D
Acq On : 27 Jan 2023 14:06
Operator : CG/JU
Sample : 01221-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-13-0118

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-BP012623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP013616.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.222	3	6	26	rVB	8600746	10153042	100.00%	17.206%
2	3.781	96	101	107	rBV	95301	121816	1.20%	0.206%
3	5.216	337	345	350	rBV	785544	1157945	11.40%	1.962%
4	5.687	418	425	434	rBV	2240526	3380818	33.30%	5.729%
5	7.293	691	698	707	rBV	1491227	2364514	23.29%	4.007%
6	8.152	837	844	851	rBV	839300	1315751	12.96%	2.230%
7	9.328	1037	1044	1053	rBV	2056732	3338735	32.88%	5.658%
8	10.981	1318	1325	1332	rBV	1004011	1746256	17.20%	2.959%
9	13.416	1731	1739	1746	rBV	5556957	8316941	81.92%	14.094%
10	14.792	1966	1973	1982	rBV	1442089	2209229	21.76%	3.744%
11	16.145	2197	2203	2208	rBV	485153	662345	6.52%	1.122%
12	16.275	2219	2225	2244	rBV	3718258	5765644	56.79%	9.771%
13	16.533	2264	2269	2279	rVB2	75939	134619	1.33%	0.228%
14	17.545	2435	2441	2454	rBV	1693574	2415176	23.79%	4.093%
15	18.398	2581	2586	2594	rBV	390268	592664	5.84%	1.004%
16	19.622	2790	2794	2805	rBV	187150	296224	2.92%	0.502%
17	20.074	2866	2871	2882	rVB	7649290	9598877	94.54%	16.267%
18	21.298	3076	3079	3085	rBV2	121143	147867	1.46%	0.251%
19	21.621	3129	3134	3139	rBV	1800947	2447559	24.11%	4.148%
20	22.951	3358	3360	3368	rVB	147962	213403	2.10%	0.362%
21	24.215	3568	3575	3586	rVB2	1222678	2629565	25.90%	4.456%

Sum of corrected areas: 59008990

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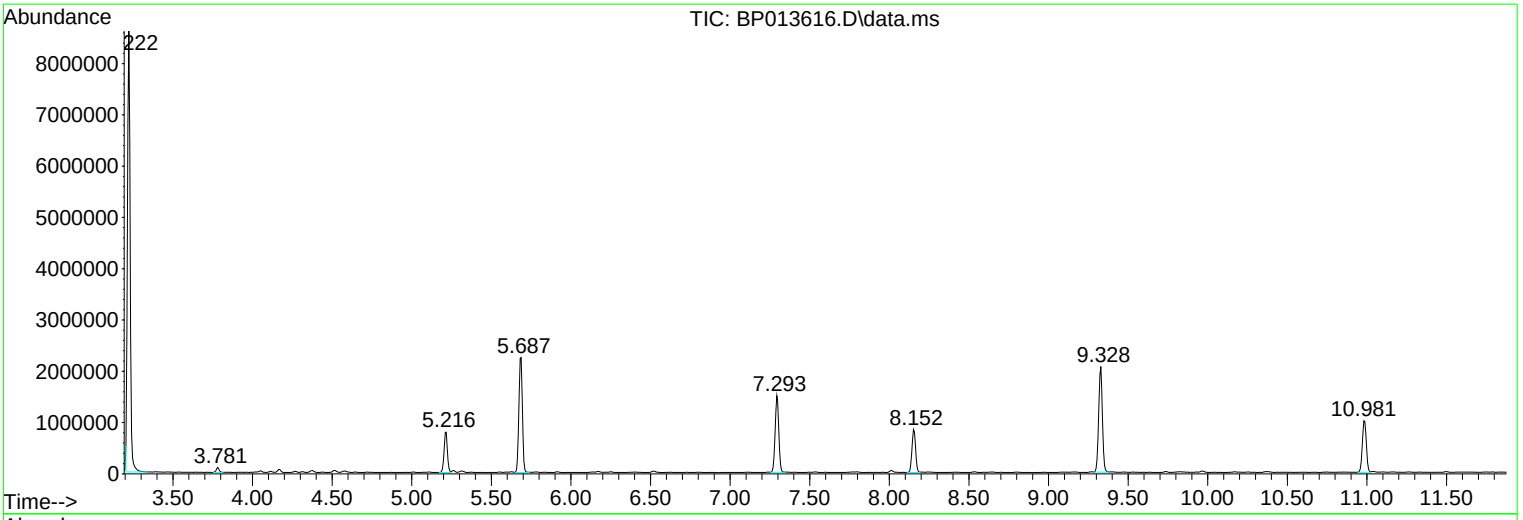
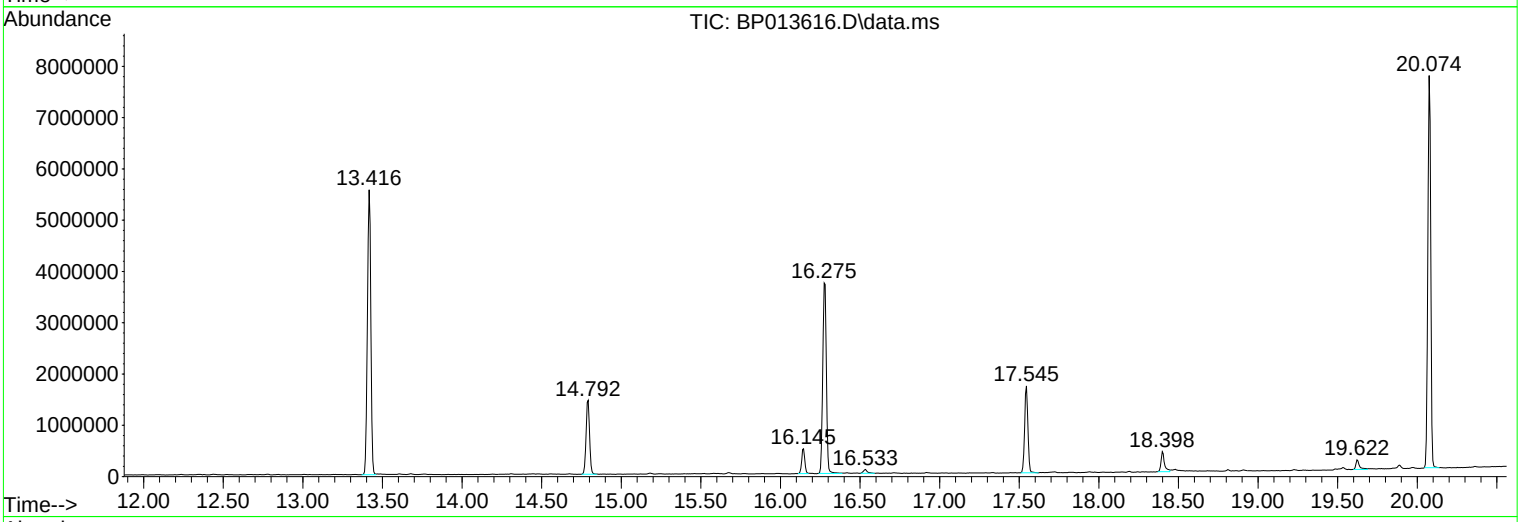
Misc :
ALS Vial : 9 Sample Multiplier: 1

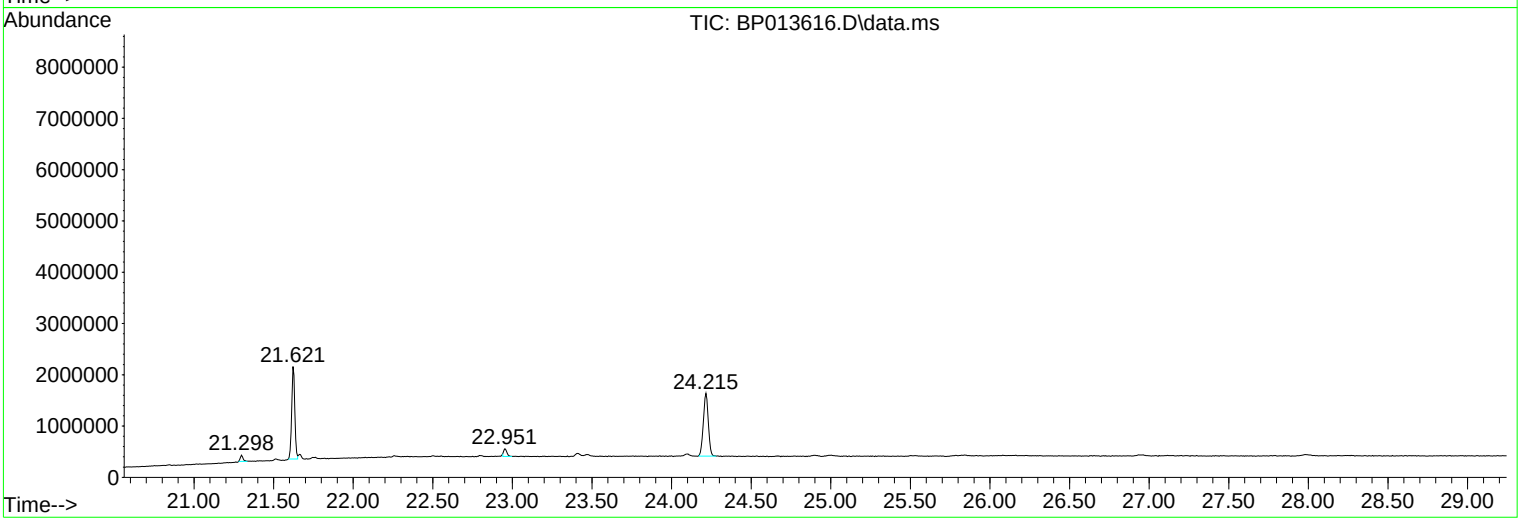
Instrument :
BNA_P
ClientSampleId :
MW-13-0118

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP012623.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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Data File : BP013616.D
Acq On : 27 Jan 2023 14:06
Operator : CG/JU
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

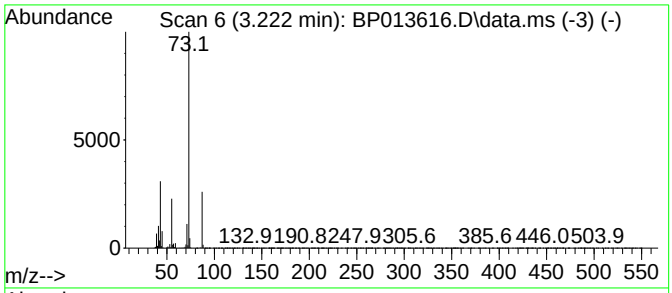
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

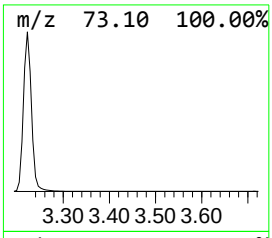
****

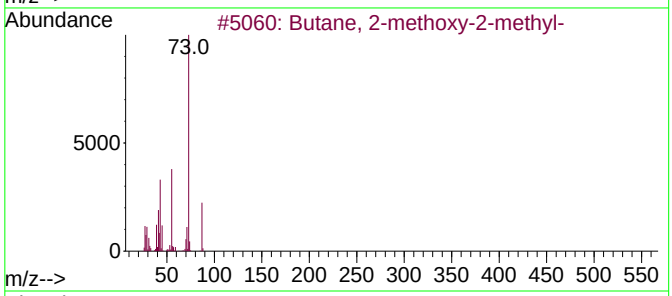
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

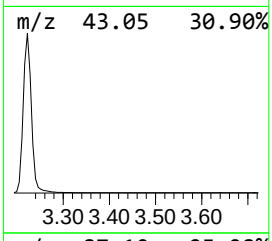
R.T.	EstConc	Area	Relative to ISTD	R.T.
3.222	154.33 ng	10153000	1,4-Dichlorobenzene-d4	8.152

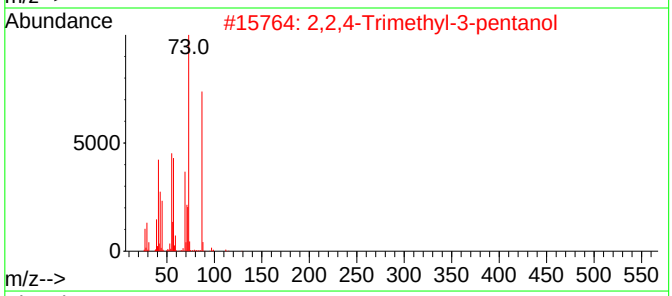
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9

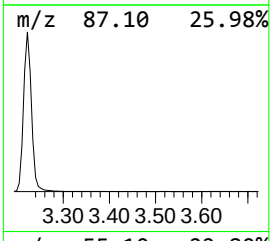


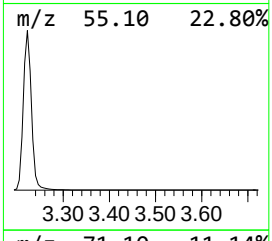


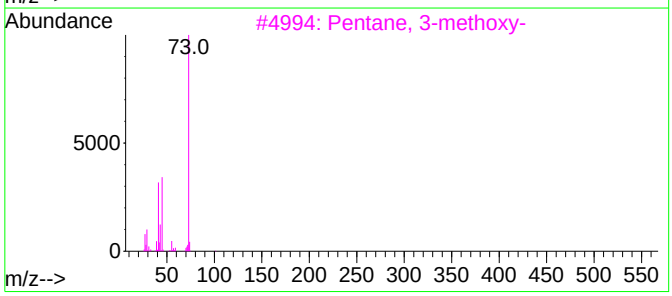


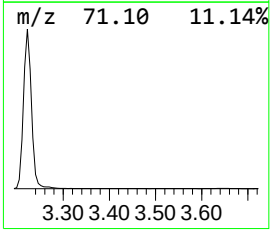












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Data File : BP013616.D
Acq On : 27 Jan 2023 14:06
Operator : CG/JU
Sample : 01221-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-13-0118

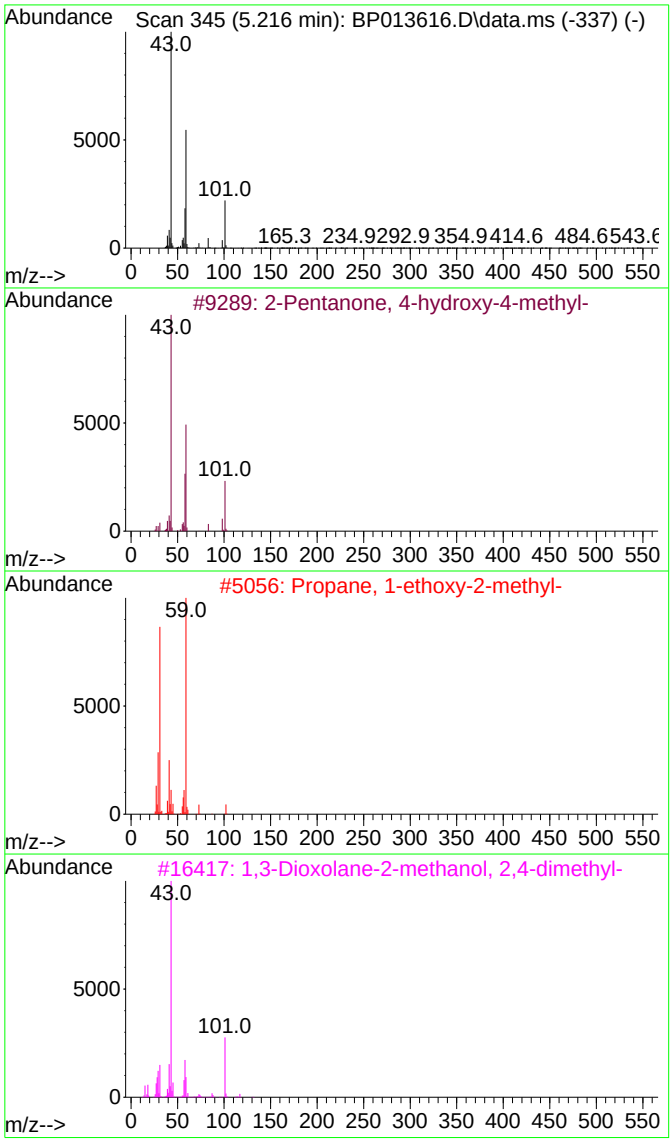
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP012623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

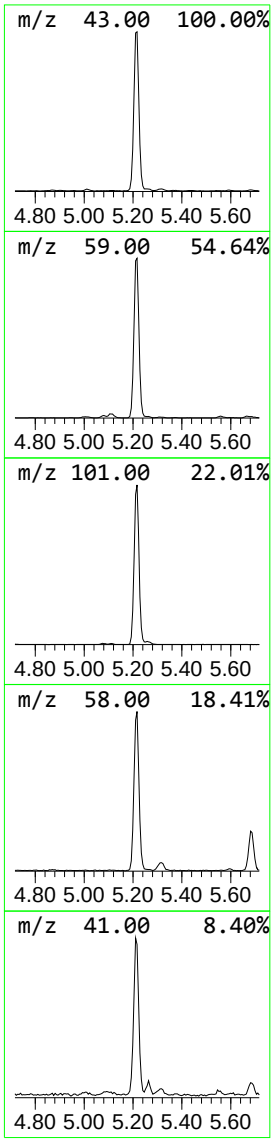
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.216	17.60 ng	1157950	1,4-Dichlorobenzene-d4	8.152

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	25
3	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	23
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	12
5	Hexanamide	115	C6H13NO	000628-02-4	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP012723\
Data File : BP013616.D
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Operator : CG/JU
Sample : 01221-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-13-0118

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP012623.M
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TIC Library : C:\Database\NIST20.L
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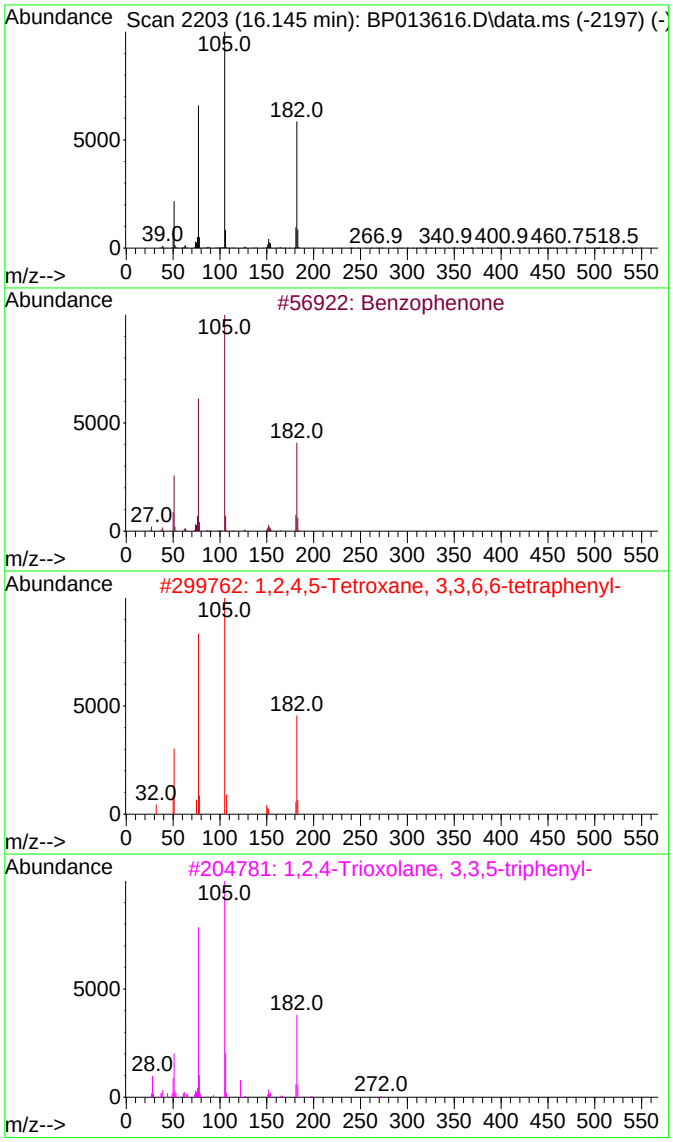
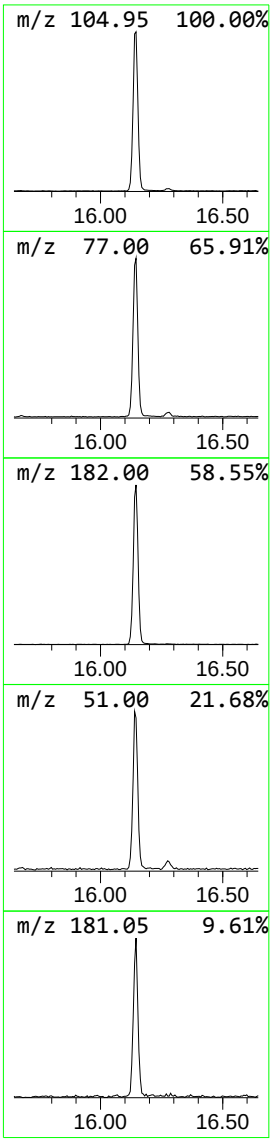
Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.145	6.00 ng	662345	Acenaphthene-d10	14.792

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	78
3	1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	50
4	Azobenzene	182	C12H10N2	000103-33-3	42
5	1,2,4-Triazolo[4,3-b]pyridazine,...	182	C7H7ClN4	028593-26-2	38





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Data File : BP013616.D
Acq On : 27 Jan 2023 14:06
Operator : CG/JU
Sample : 01221-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-13-0118

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP012623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

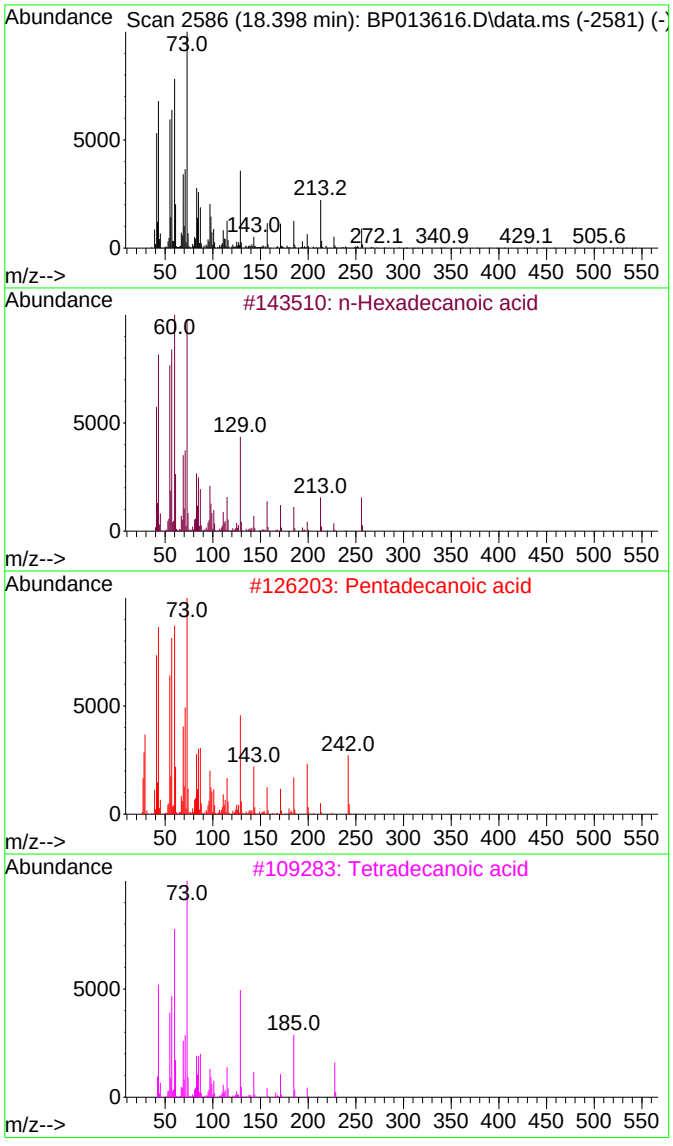
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

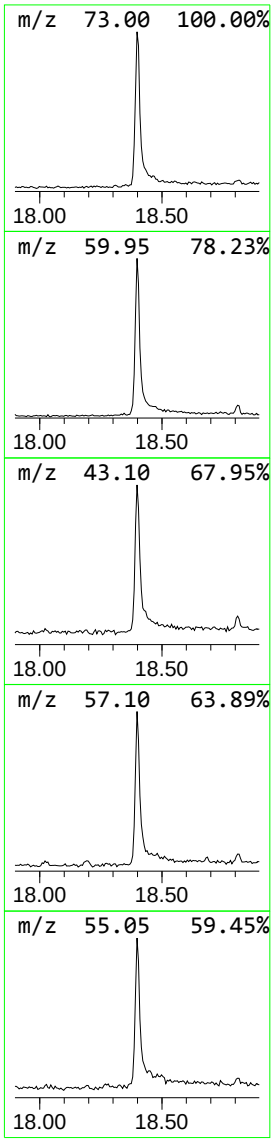
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.398	4.91 ng	592664	Phenanthrene-d10	17.545

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	92
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4	Tridecanoic acid	214	C13H26O2	000638-53-9	68
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64





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Operator : CG/JU
Sample : 01221-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-13-0118

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP012623.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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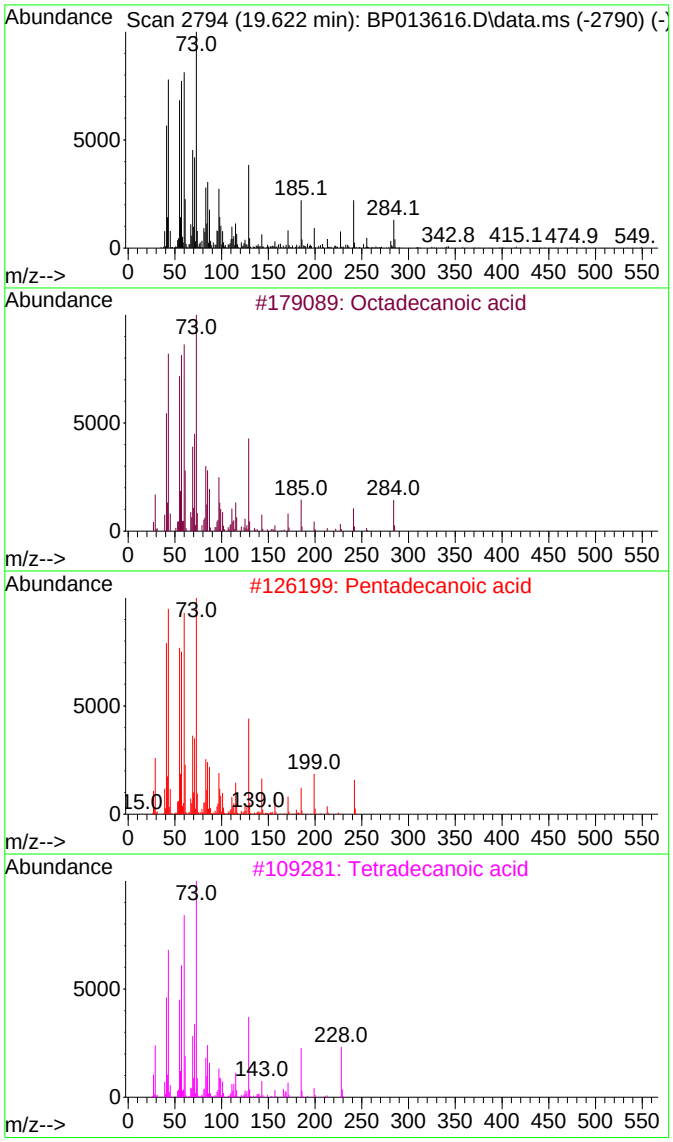
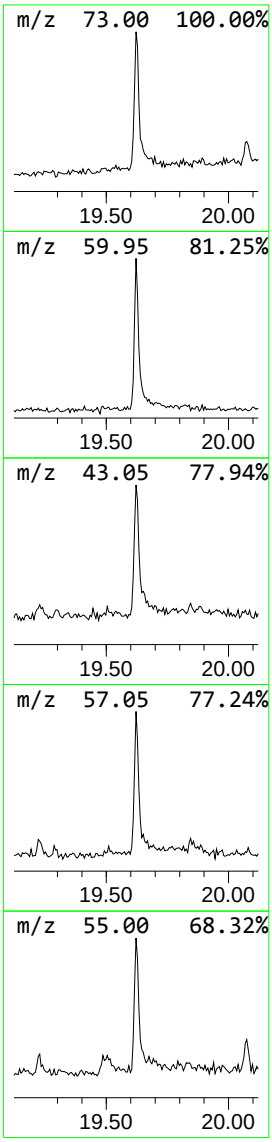
Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.622	2.42 ng	296224	Chrysene-d12	21.621

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	n-Decanoic acid	172	C10H20O2	000334-48-5	64
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	62





Tentatively Identified Compound (LSC) summary

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	3.222	154.3	ng	10153000	1	8.152	1315750	20.0
2-Pentanone, 4-...	5.216	17.6	ng	1157950	1	8.152	1315750	20.0
Benzophenone	16.145	6.0	ng	662345	3	14.792	2209230	20.0
n-Hexadecanoic ...	18.398	4.9	ng	592664	4	17.545	2415180	20.0
Octadecanoic acid	19.622	2.4	ng	296224	5	21.621	2447560	20.0