LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM061323\
Data File : BM040231.D
Acq On : 13 Jun 2023 18:49
Operator : MA/JU
Sample : 03047-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-41

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-BM061323.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM040231.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.516	36	39	51	rVB	126610	164891	1.01%	0.162%
2	4.446	192	197	209	rVB	1142782	1471419	9.05%	1.448%
3	5.063	295	302	317	rBV	4892547	6548787	40.28%	6.445%
4	5.528	375	381	398	rBV	2126938	2990971	18.40%	2.943%
5	6.151	481	487	497	rBV	575243	805975	4.96%	0.793%
6	7.134	645	654	672	rVB	1210278	1902532	11.70%	1.872%
7	7.975	790	797	805	rBV	2218115	3415090	21.01%	3.361%
8	9.145	988	996	1005	rBV	4072534	6512091	40.06%	6.409%
9	10.792	1268	1276	1284	rBV	2961762	4872199	29.97%	4.795%
10	13.245	1685	1693	1701	rBV	10144252	14300707	87.97%	14.074%
11	14.616	1919	1926	1941	rBV	4224395	6004166	36.93%	5.909%
12	15.974	2147	2157	2162	rBV	2486570	3346243	20.58%	3.293%
13	16.104	2172	2179	2193	rBV	4276987	5933734	36.50%	5.839%
14	16.533	2248	2252	2259	rVB	191281	255019	1.57%	0.251%
15	17.362	2386	2393	2399	rBV	4682798	6421478	39.50%	6.319%
16	18.256	2539	2545	2553	rBV	2211464	3221836	19.82%	3.171%
17	18.327	2554	2557	2566	rVB	215162	379303	2.33%	0.373%
18	19.527	2756	2761	2781	rBV	1283593	2331739	14.34%	2.295%
19	19.980	2832	2838	2849	rBV	13372753	16256582	100.00%	15.998%
20	21.233	3047	3051	3061	rBV	2149495	2729874	16.79%	2.687%
21	21.444	3084	3087	3091	rVB	239177	262166	1.61%	0.258%
22	21.539	3097	3103	3107	rBV	4439042	5797307	35.66%	5.705%
23	23.968	3510	3516	3529	rVB	2828660	5689993	35.00%	5.600%

Sum of corrected areas: 101614102

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM061323\
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Misc :
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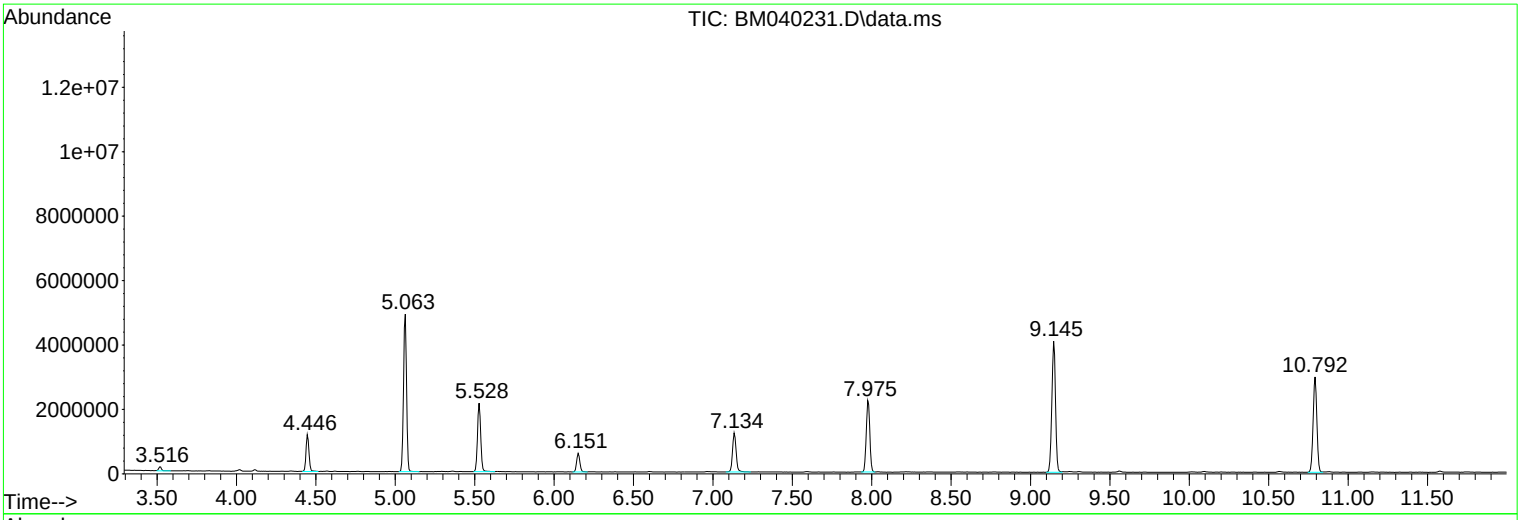
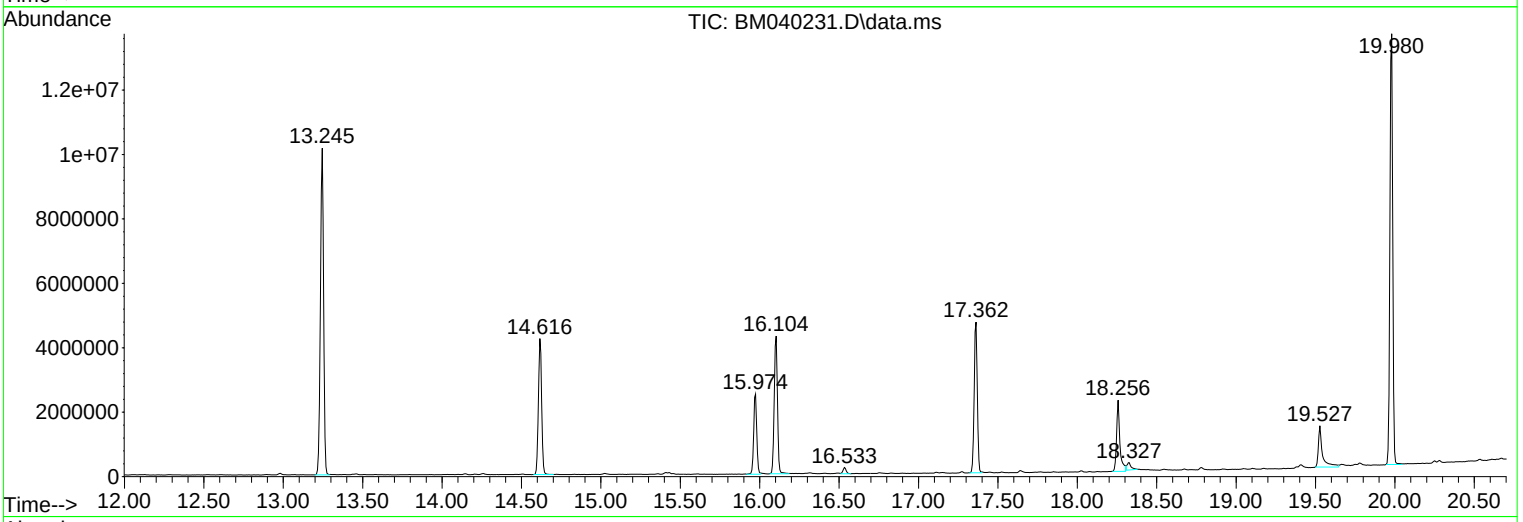
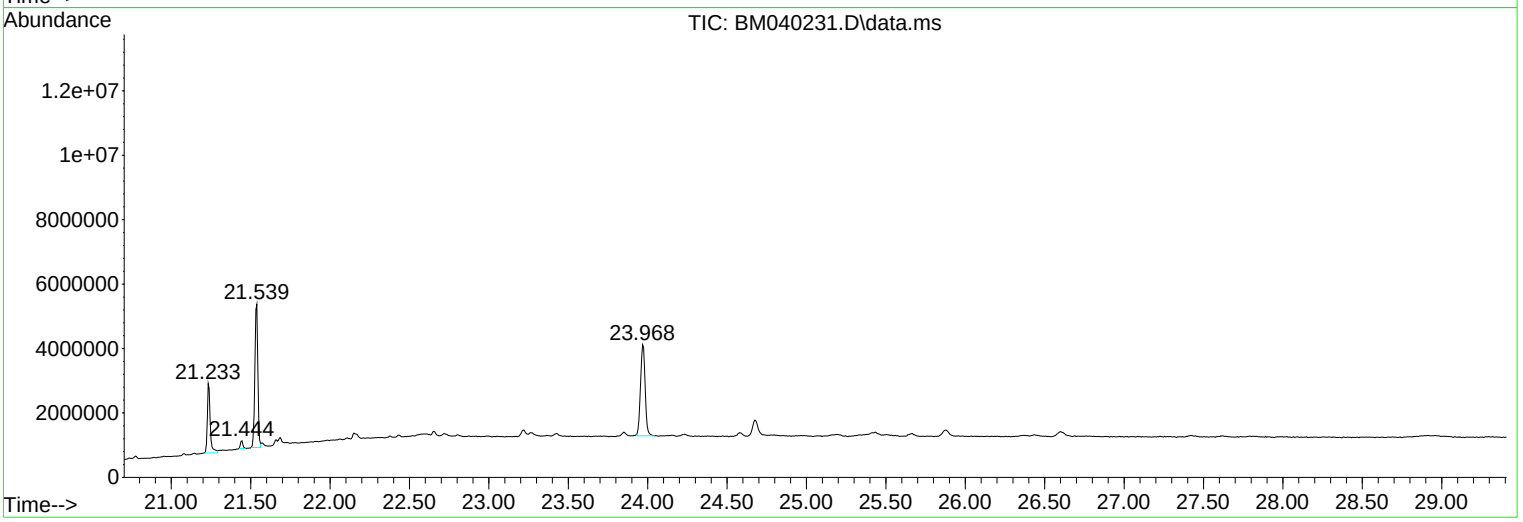
Instrument :
BNA_M
ClientSampleId :
MW-41

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM061323.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 : BM040231.D
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

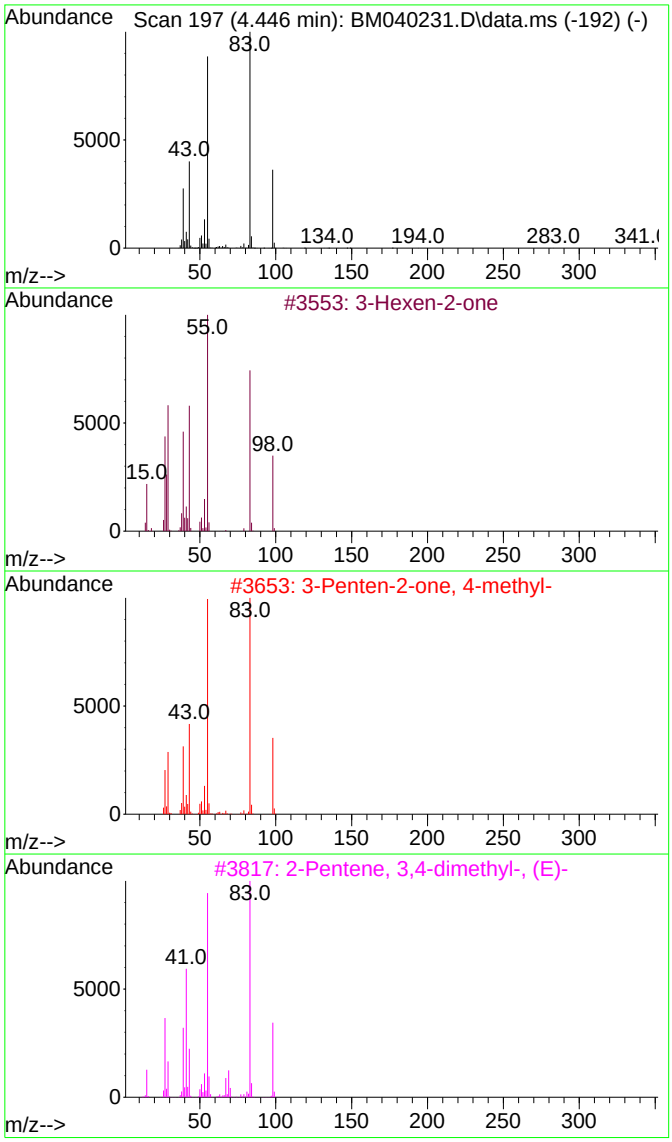
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

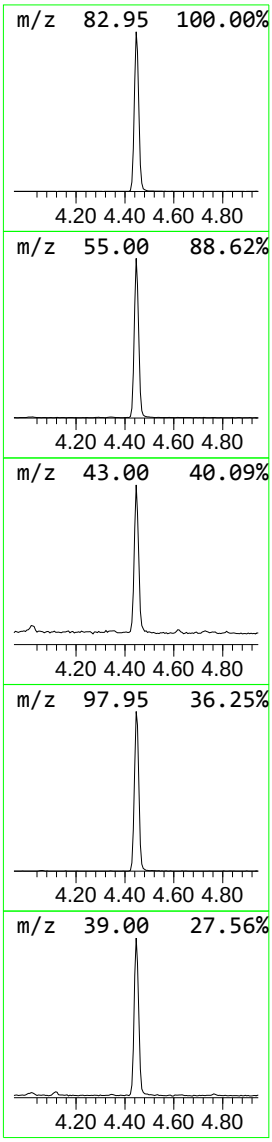
****

Peak Number 1 3-Hexen-2-one Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.446	8.62 ng	1471420	1,4-Dichlorobenzene-d4	7.975

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-2-one	98	C6H10O	000763-93-9	91
2	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
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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Sample : 03047-09
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Instrument :
BNA_M
ClientSampleId :
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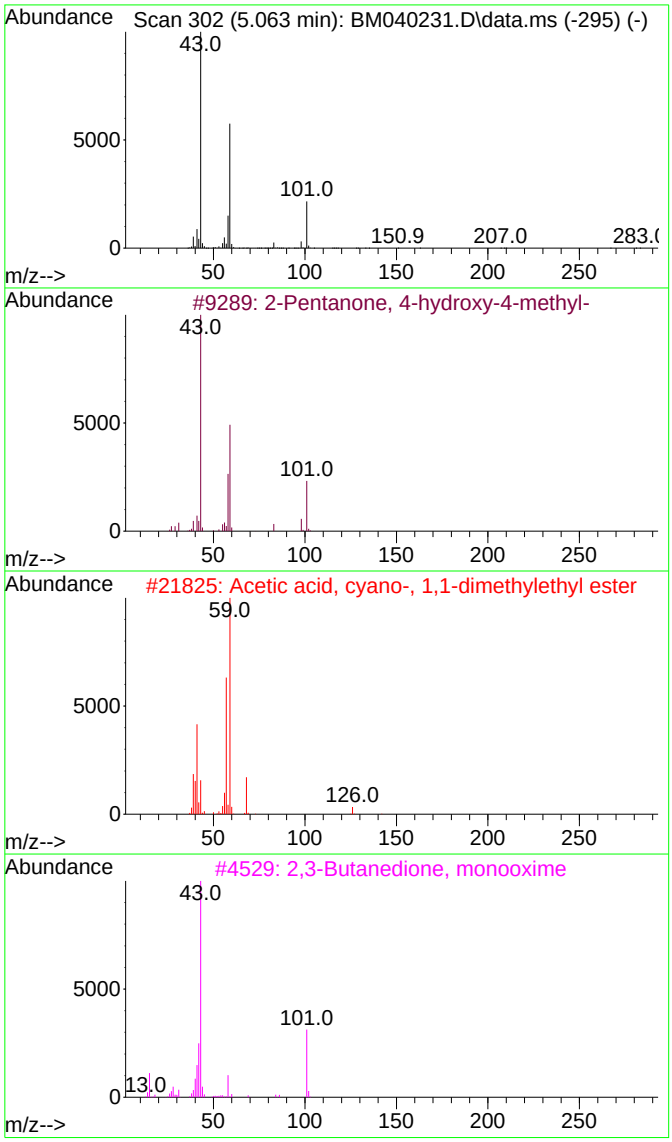
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

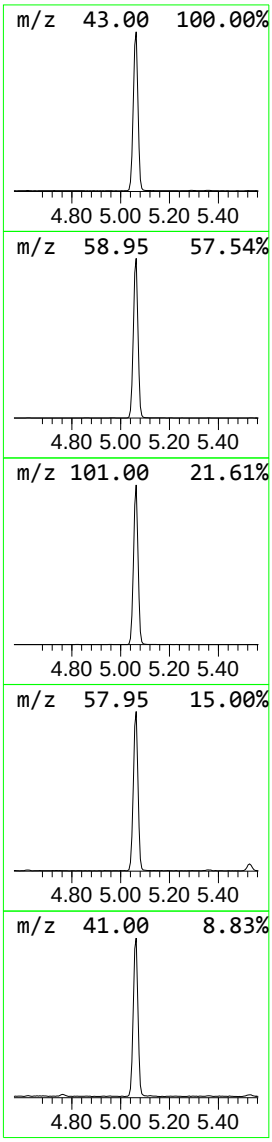
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.063	38.35 ng	6548790	1,4-Dichlorobenzene-d4	7.975

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Acq On : 13 Jun 2023 18:49
Operator : MA/JU
Sample : 03047-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-41

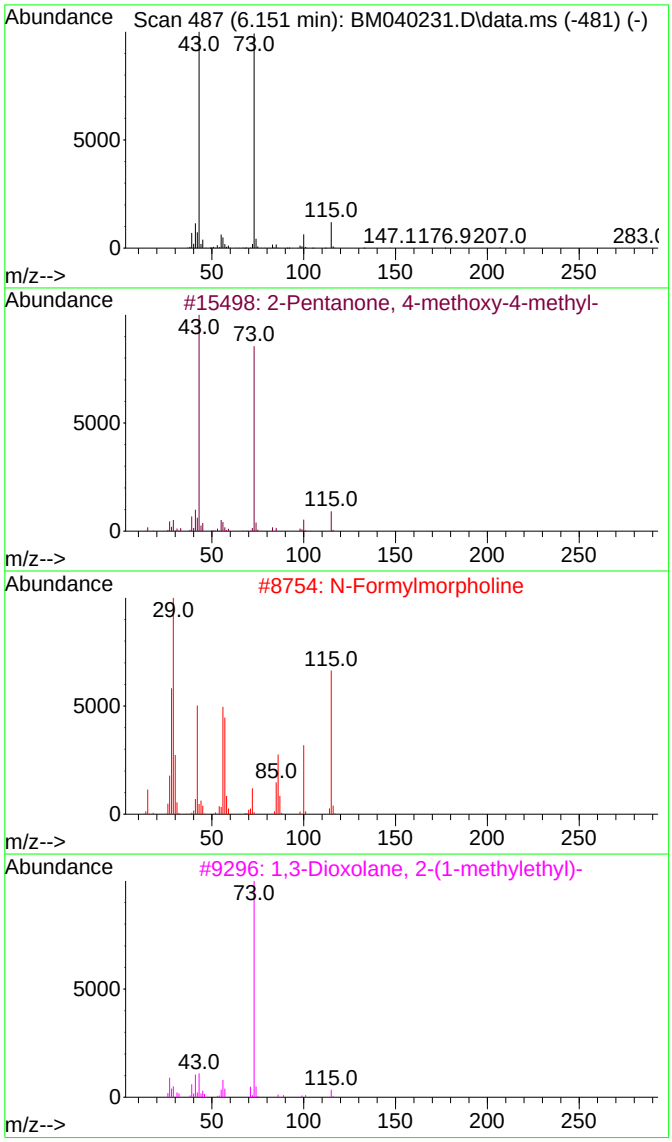
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM061323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

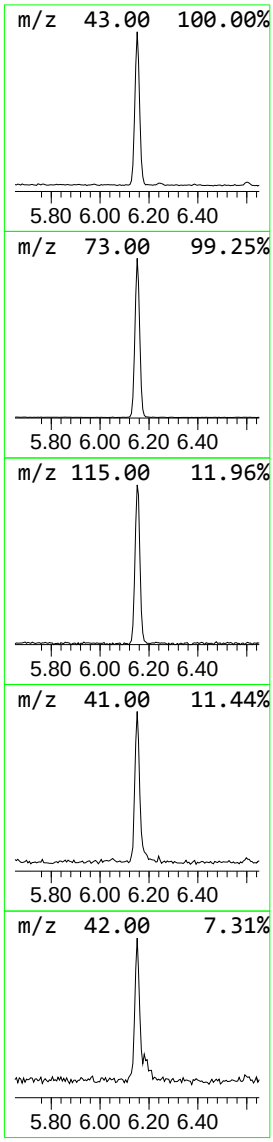
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.151	4.72 ng	805975	1,4-Dichlorobenzene-d4	7.975

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	N-Formylmorpholine	115	C5H9NO2	004394-85-8	10
3	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	10
4	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9





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Data File : BM040231.D
Acq On : 13 Jun 2023 18:49
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Sample : 03047-09
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Instrument :
BNA_M
ClientSampleId :
MW-41

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM061323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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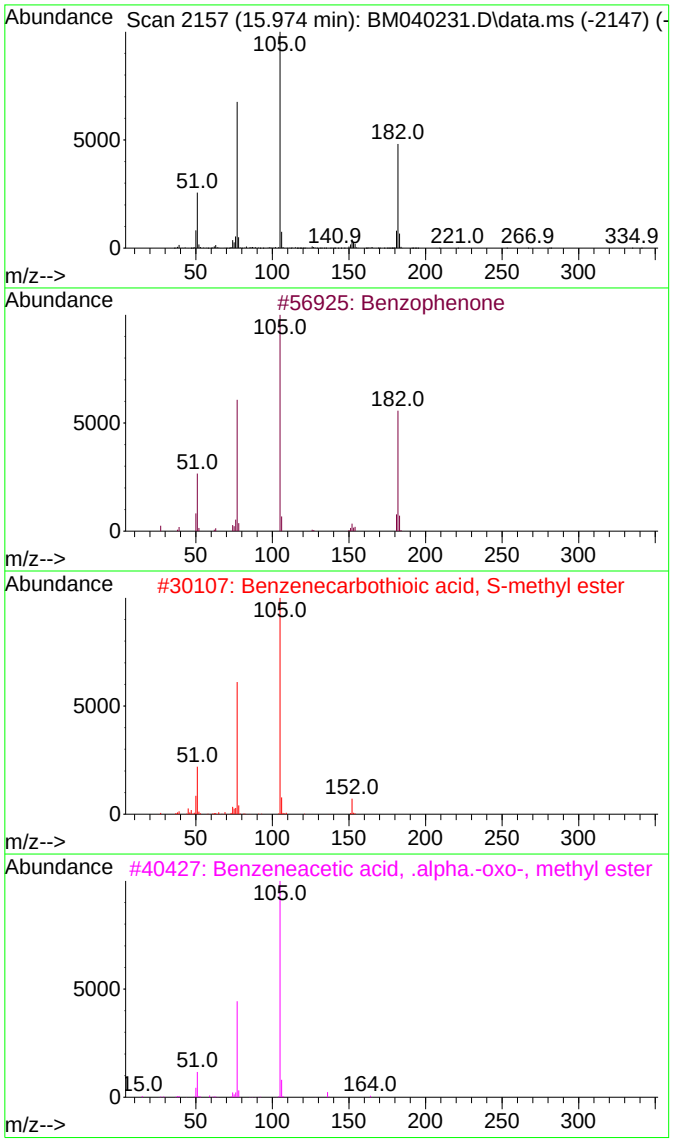
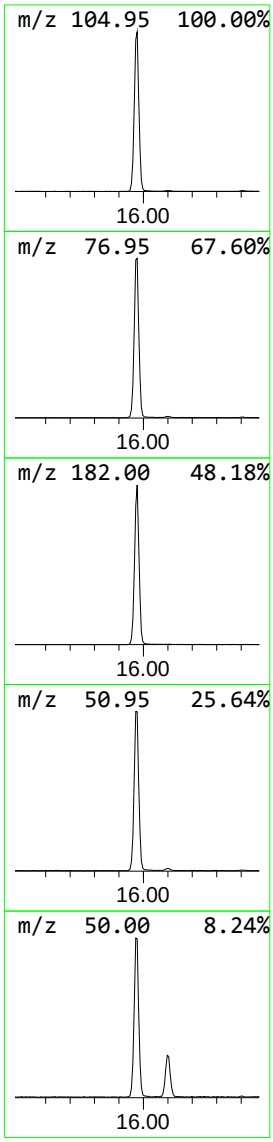
****

Peak Number 4 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.974	11.15 ng	3346240	Acenaphthene-d10	14.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	52
3	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	49
4	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
5	Benzoylformic acid	150	C8H6O3	000611-73-4	47





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BNA_M
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM061323.M
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TIC Library : C:\Database\NIST20.L
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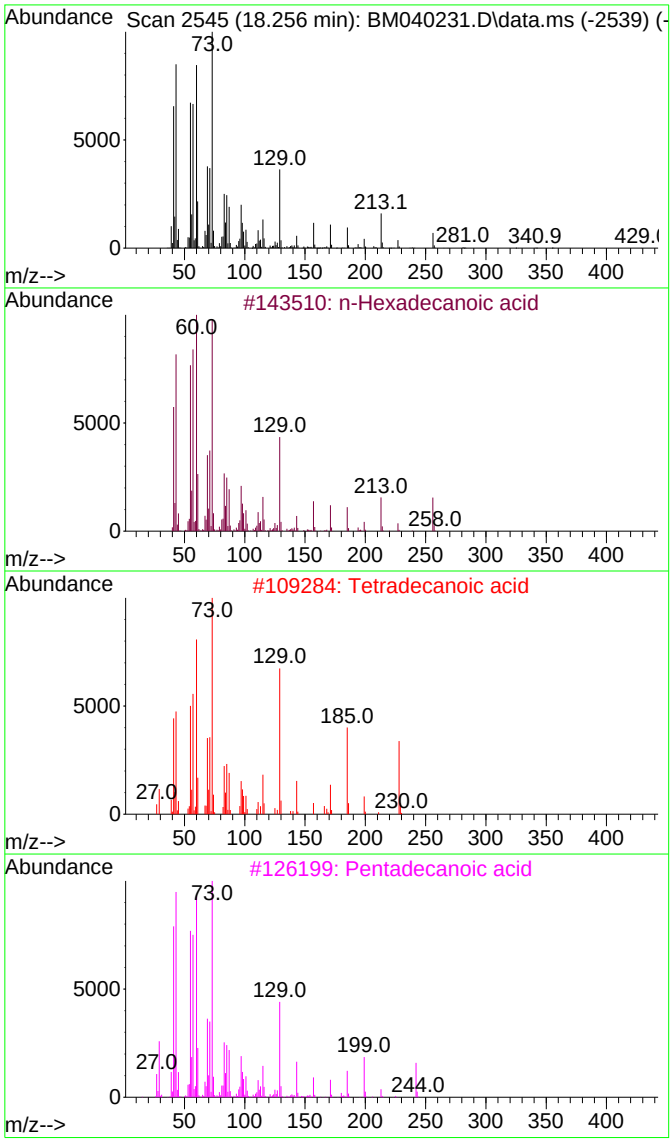
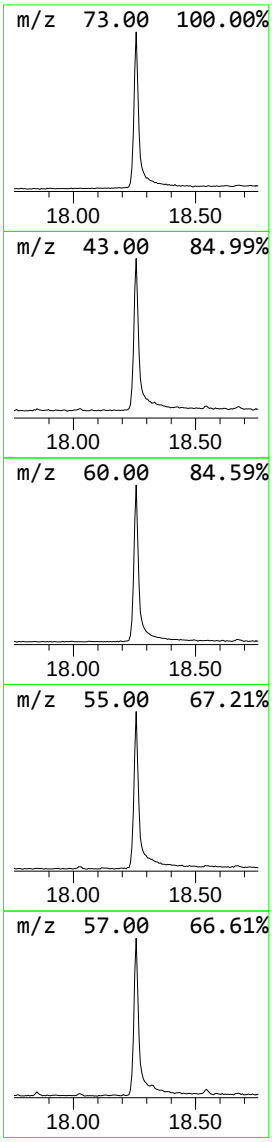
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.256	10.03 ng	3221840	Phenanthrene-d10	17.362

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	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tridecanoic acid	214	C13H26O2	000638-53-9	87
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64





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TIC Library : C:\Database\NIST20.L
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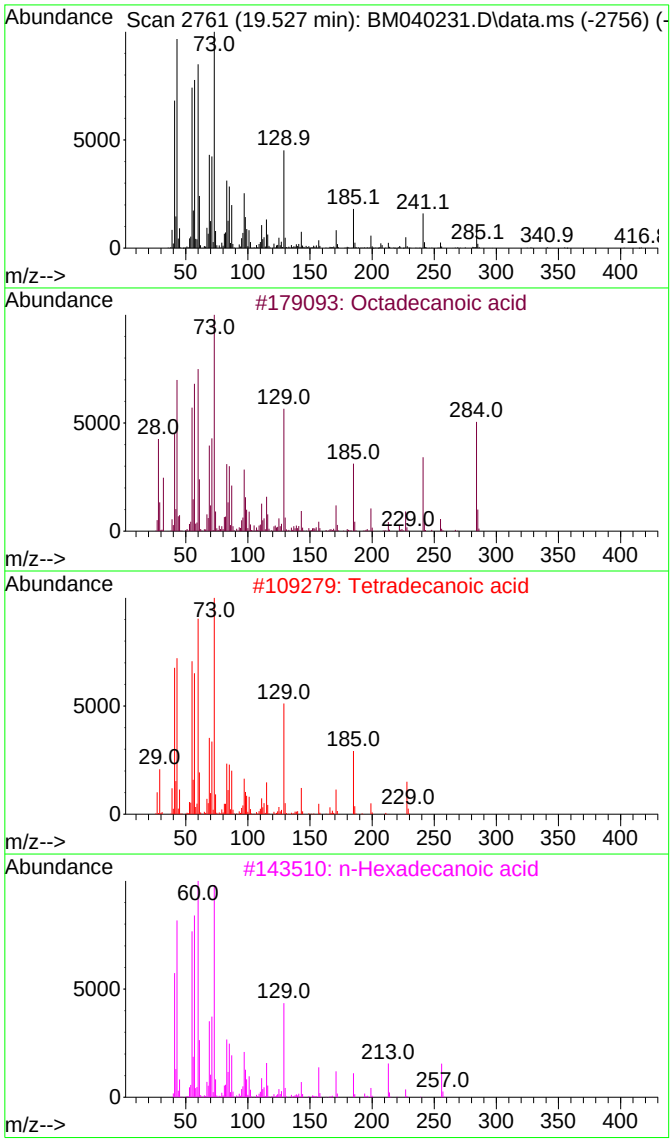
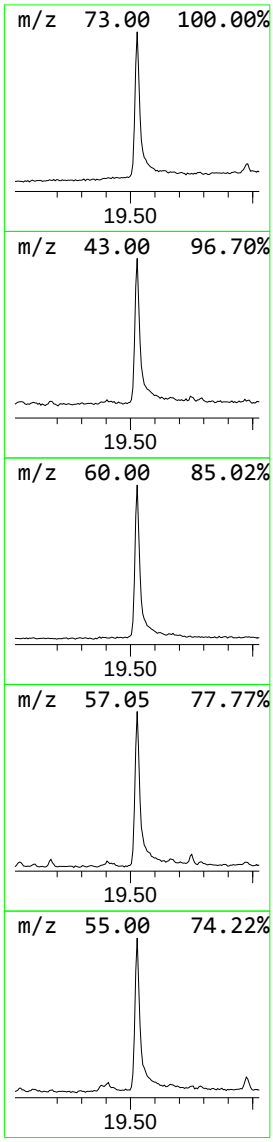
****

Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.527	8.04 ng	2331740	Chrysene-d12	21.539

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	93
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87





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

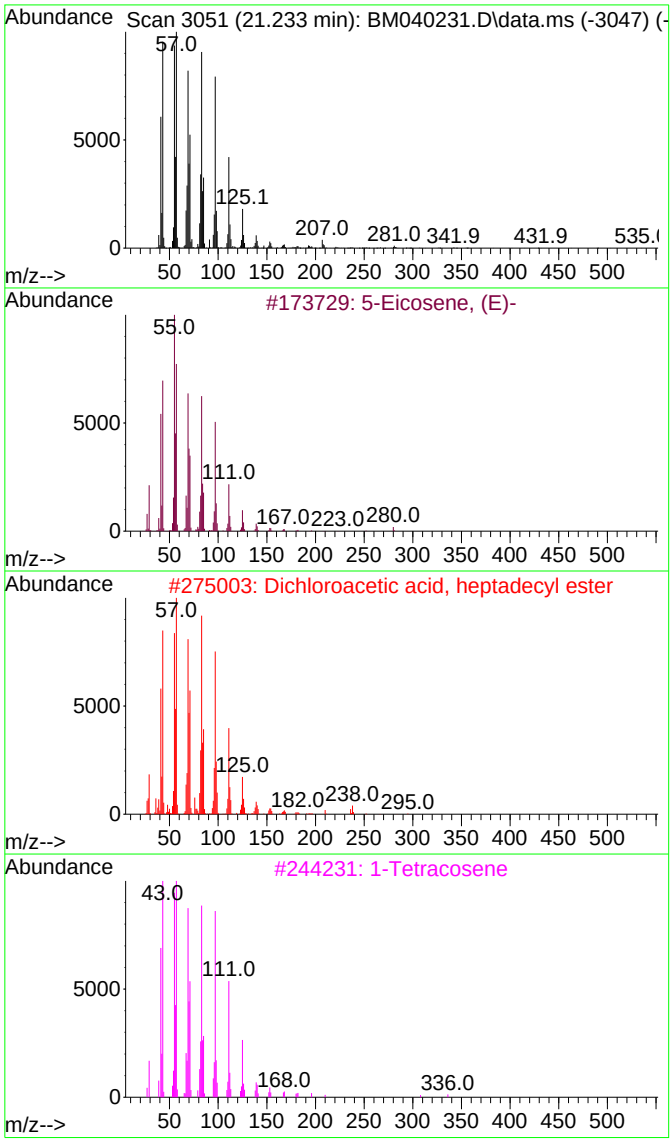
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

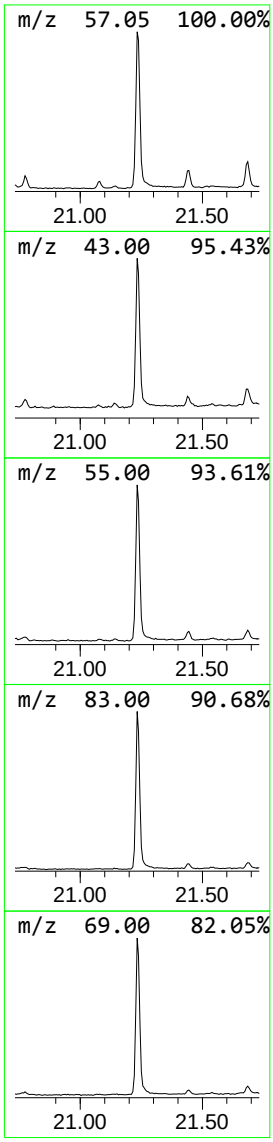
****

Peak Number 7 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.233	9.42 ng	2729870	Chrysene-d12	21.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	98
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
3	1-Tetracosene	336	C24H48	010192-32-2	94
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94





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-Hexen-2-one	4.446	8.6	ng	1471420	1	7.975	3415090	20.0
2-Pentanone, 4-...	5.063	38.4	ng	6548790	1	7.975	3415090	20.0
2-Pentanone, 4-...	6.151	4.7	ng	805975	1	7.975	3415090	20.0
Benzophenone	15.974	11.2	ng	3346240	3	14.616	6004170	20.0
n-Hexadecanoic ...	18.256	10.0	ng	3221840	4	17.362	6421480	20.0
Octadecanoic acid	19.527	8.0	ng	2331740	5	21.539	5797310	20.0
5-Eicosene, (E)-	21.233	9.4	ng	2729870	5	21.539	5797310	20.0