LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031324\
Data File : BM044608.D
Acq On : 13 Mar 2024 21:36
Operator : MA/JU
Sample : PB159537BL
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB159537BL

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-BM031324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM044608.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.963	145	149	157	rVB	202188	256284	2.85%	0.495%
2	4.281	198	203	212	rVB	171999	232647	2.59%	0.449%
3	4.869	297	303	316	rBV	1168008	1638996	18.21%	3.164%
4	5.310	371	378	391	rBV	2962369	4255597	47.29%	8.216%
5	6.881	637	645	658	rBV	2605014	4146674	46.08%	8.005%
6	7.704	778	785	791	rBV	757014	1225036	13.61%	2.365%
7	8.863	974	982	993	rBV	2302471	3828491	42.54%	7.391%
8	10.480	1248	1257	1269	rBV	946966	1633442	18.15%	3.153%
9	12.963	1672	1679	1695	rBV	4950760	7558484	83.99%	14.592%
10	14.345	1907	1914	1923	rBV	1255211	1904227	21.16%	3.676%
11	15.845	2162	2169	2178	rBV	2309182	3487546	38.76%	6.733%
12	16.368	2254	2258	2269	rVB2	44152	100881	1.12%	0.195%
13	17.098	2376	2382	2397	rBV	1373172	2045720	22.73%	3.949%
14	19.227	2739	2744	2752	rVV2	123183	260581	2.90%	0.503%
15	19.297	2752	2756	2764	rVB	93578	152242	1.69%	0.294%
16	19.744	2826	2832	2838	rBV	7015743	8998841	100.00%	17.373%
17	21.297	3091	3096	3100	rBV	1699827	2491886	27.69%	4.811%
18	21.333	3100	3102	3121	rVB2	559028	1298724	14.43%	2.507%
19	21.786	3173	3179	3183	rBV3	476932	1059642	11.78%	2.046%
20	21.838	3184	3188	3208	rVB4	719692	2708590	30.10%	5.229%
21	23.544	3472	3478	3486	rVB	1307988	2513428	27.93%	4.852%

Sum of corrected areas: 51797959

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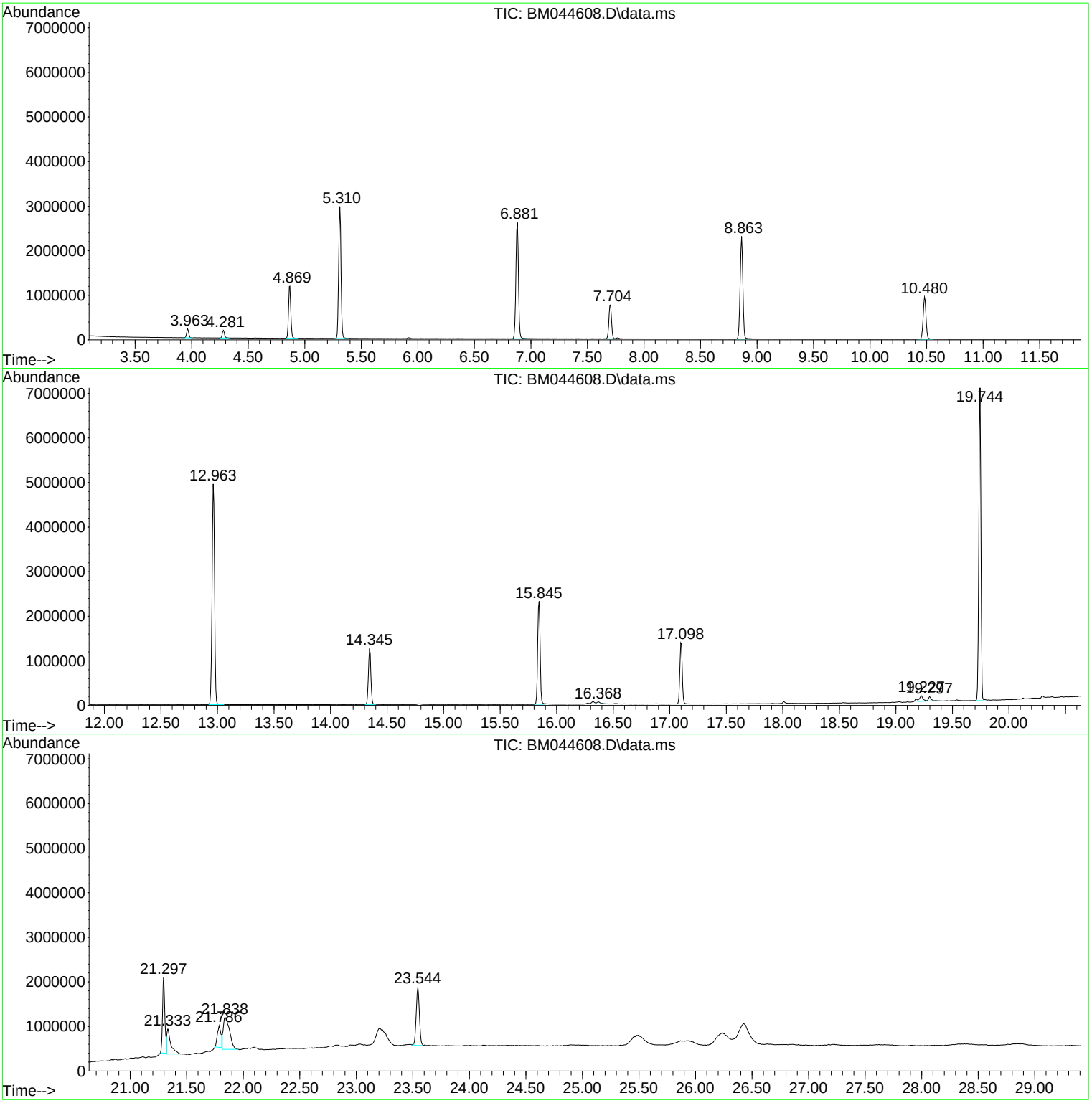
PB159537BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031324.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 : BM044608.D
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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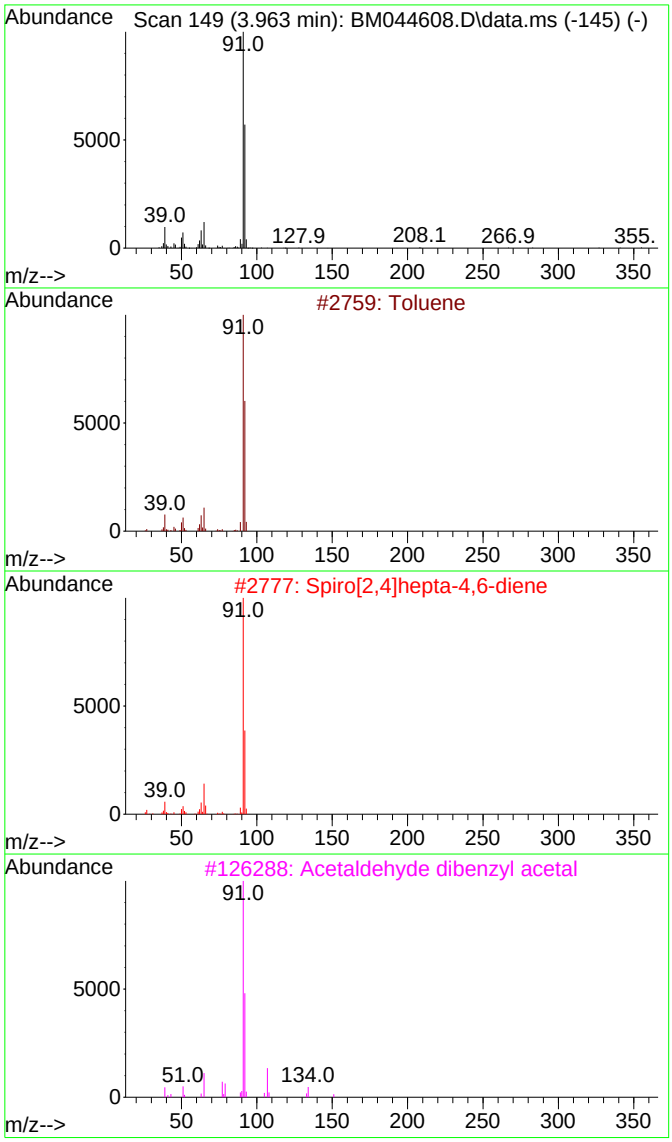
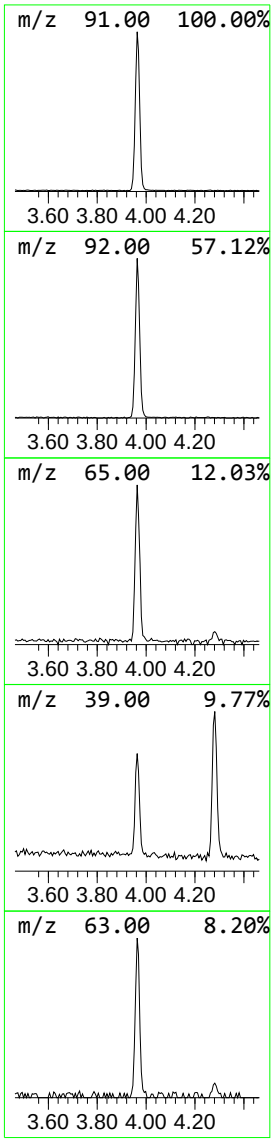
Peak Number 1 Toluene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.963	4.18 ng	256284	1,4-Dichlorobenzene-d4	7.704

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Toluene	92	C7H8	000108-88-3	94
2	Spiro[2,4]hepta-4,6-diene	92	C7H8	000765-46-8	87
3	Acetaldehyde dibenzyl acetal	242	C16H18O2	1000431-44-3	72
4	Cyclobutene, 2-propenylidene-	92	C7H8	052097-85-5	72
5	Benzene, (butoxymethyl)-	164	C11H16O	000588-67-0	72





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

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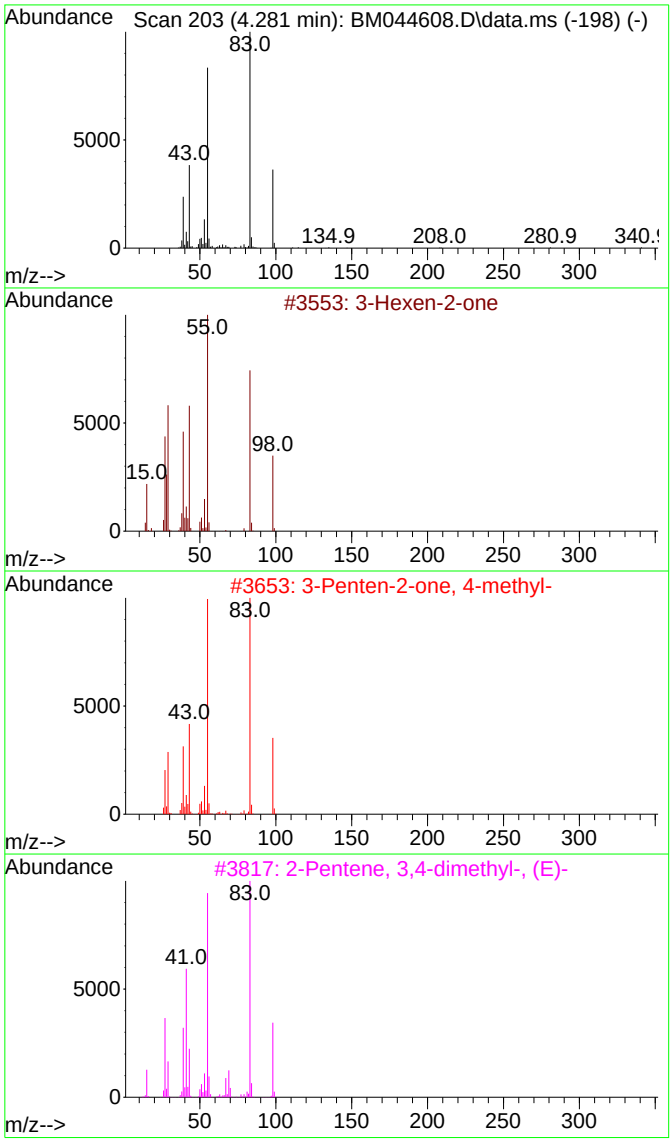
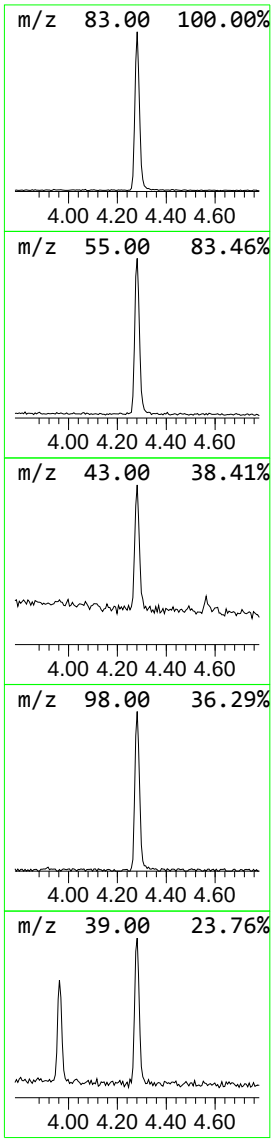
Peak Number 2 3-Hexen-2-one Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.281	3.80 ng	232647	1,4-Dichlorobenzene-d4	7.704

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-2-one	98	C6H10O	000763-93-9	90
2	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	87
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4	Cyclohexane, methyl-	98	C7H14	000108-87-2	80
5	2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	80





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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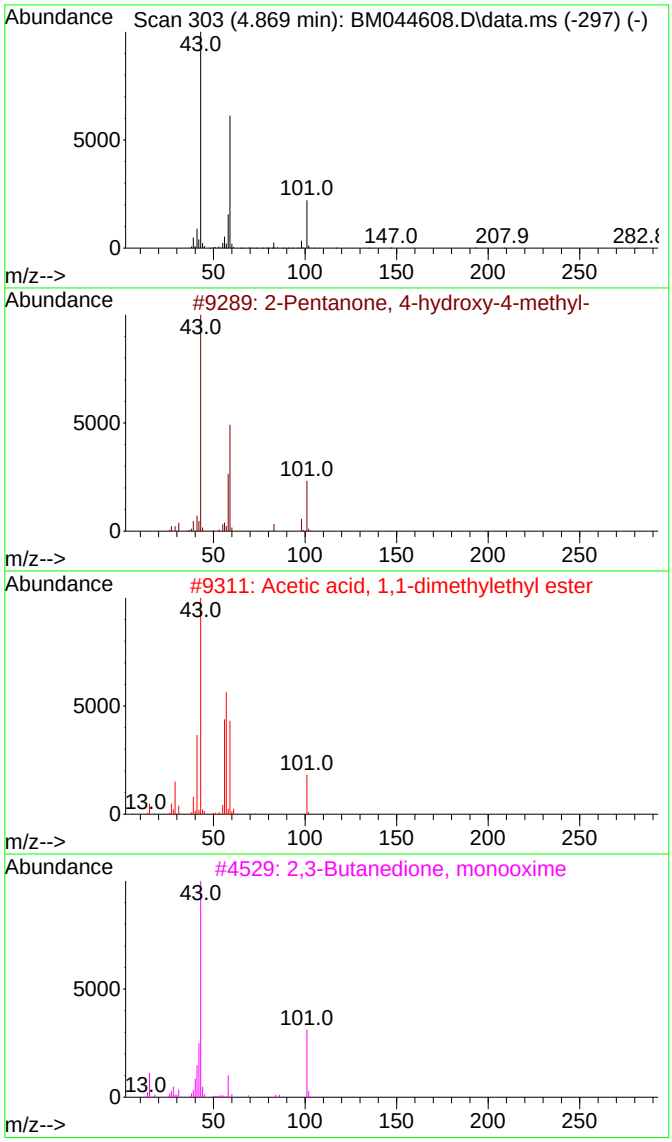
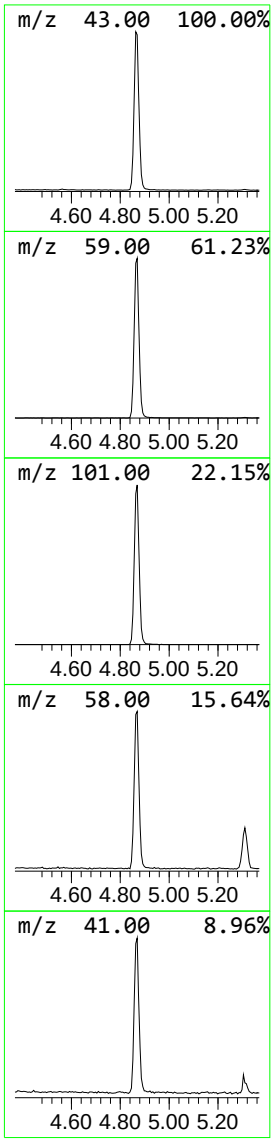
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.869	26.76 ng	1639000	1,4-Dichlorobenzene-d4	7.704

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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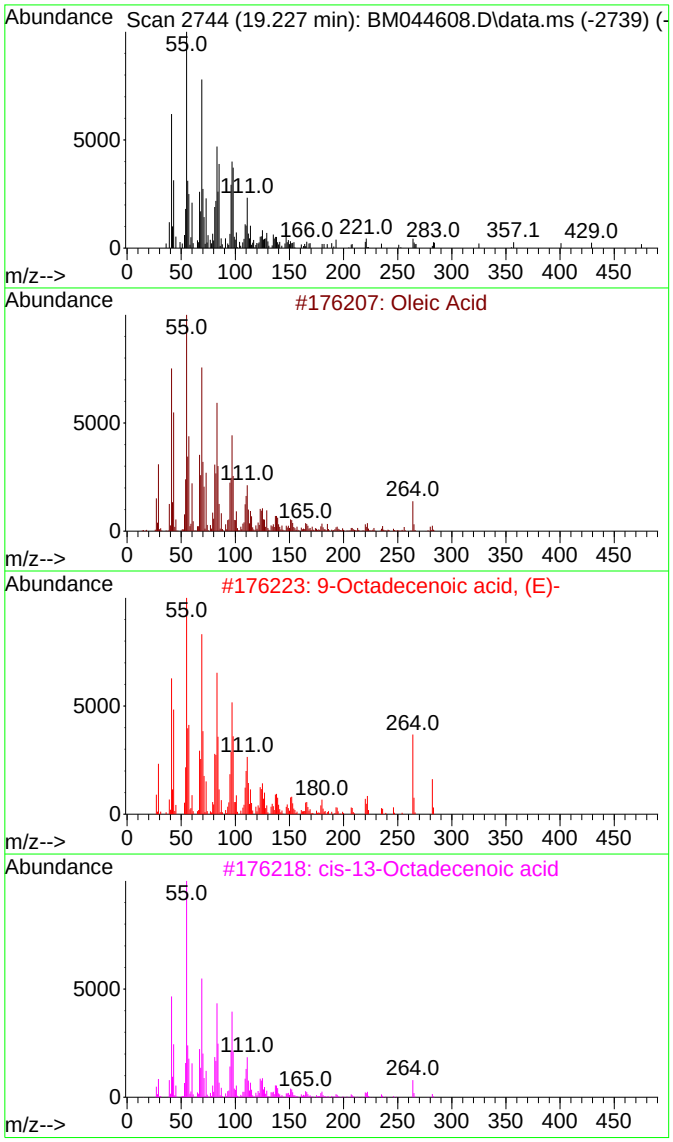
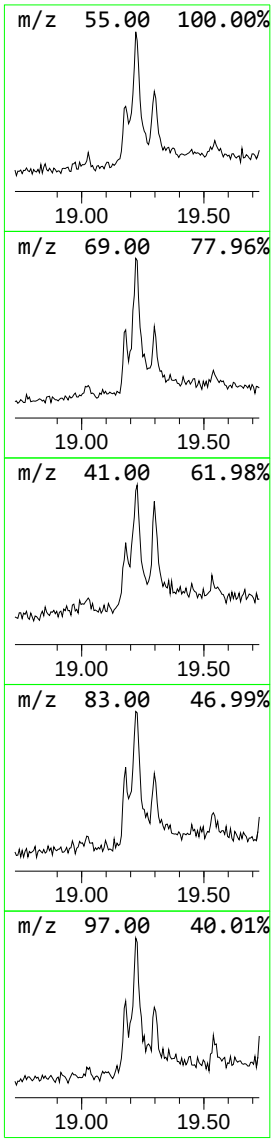
Peak Number 4 Oleic Acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.227	2.09 ng	260581	Chrysene-d12	21.297

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oleic Acid	282	C18H34O2	000112-80-1	93
2	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	92
3	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	87
4	13-Octadecenal, (Z)-	266	C18H34O	058594-45-9	64
5	6-Octadecenoic acid, (Z)-	282	C18H34O2	000593-39-5	47





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031324.M
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TIC Library : C:\Database\NIST20.L
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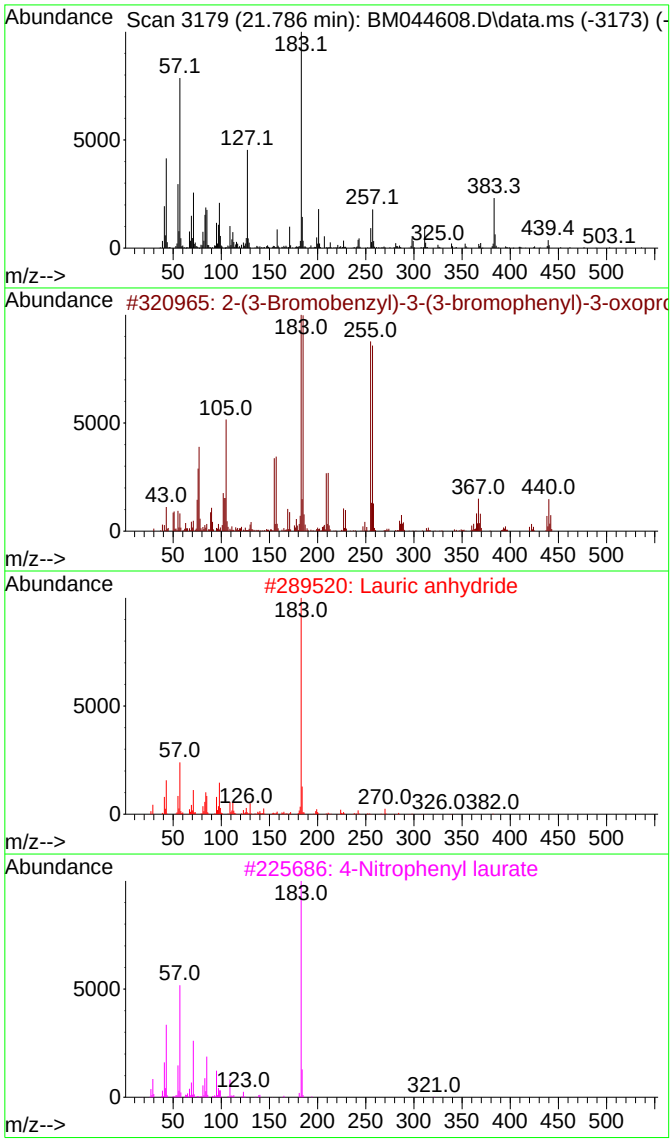
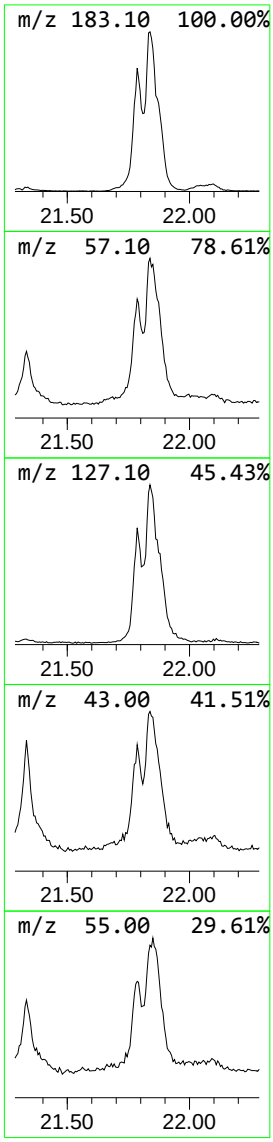
Peak Number 5 unknown21.785 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.785	8.50 ng	1059640	Chrysene-d12	21.297

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(3-Bromobenzyl)-3-(3-bromophen...	438	C18H16Br2O3	1000202-01-4	45
2	Lauric anhydride	382	C24H46O3	000645-66-9	38
3	4-Nitrophenyl laurate	321	C18H27NO4	001956-11-2	38
4	Dodecanoic acid, 2,4,5-trichloro...	378	C18H25Cl3O2	1000360-54-9	38
5	Dodecanoic acid, 1-(hydroxymethy...	456	C27H52O5	017598-94-6	37





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TIC Library : C:\Database\NIST20.L
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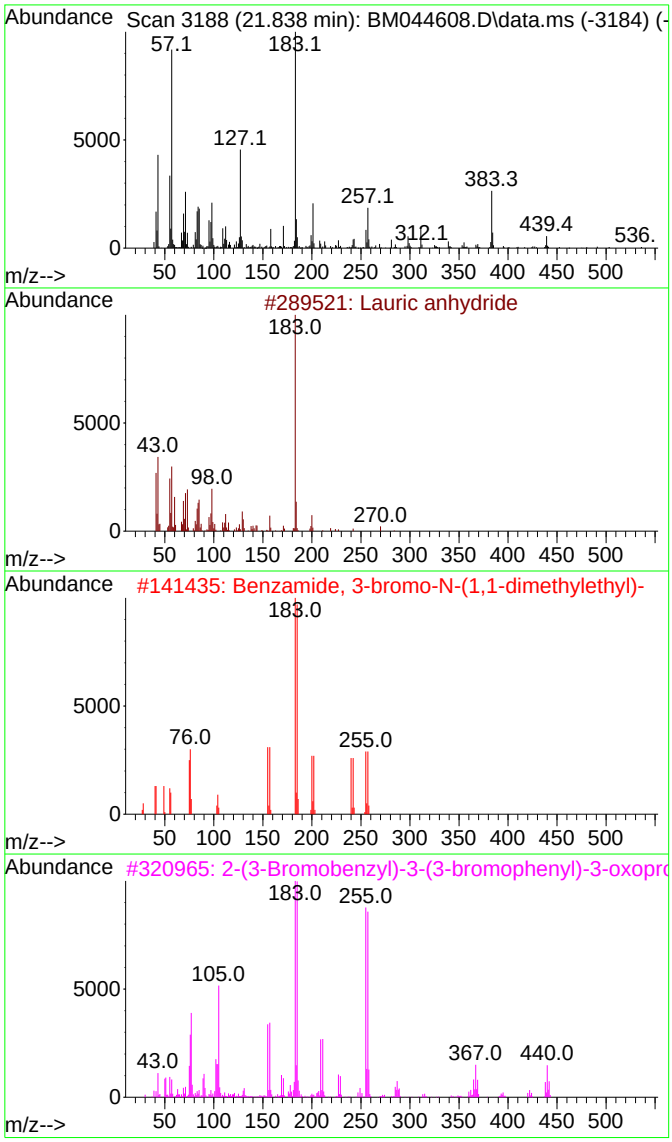
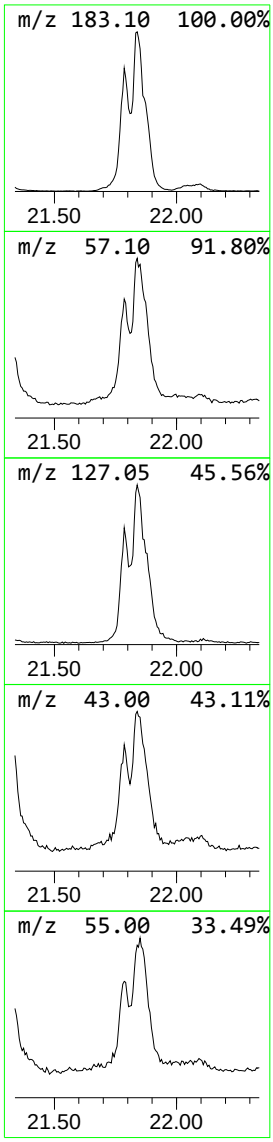
Peak Number 6 unknown21.839 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.839	21.74 ng	2708590	Chrysene-d12	21.297

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Lauric anhydride	382	C24H46O3	000645-66-9	46
2	Benzamide, 3-bromo-N-(1,1-dimeth...	255	C11H14BrNO	042498-39-5	42
3	2-(3-Bromobenzyl)-3-(3-bromophen...	438	C18H16Br2O3	1000202-01-4	42
4	Fumaric acid, hexyl 4-methylpent...	284	C16H28O4	1000348-32-0	32
5	Dodecanoic acid, 2,4,5-trichloro...	378	C18H25Cl3O2	1000360-54-9	30





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Toluene	3.963	4.2	ng	256284	1	7.704	1225040	20.0
3-Hexen-2-one	4.281	3.8	ng	232647	1	7.704	1225040	20.0
2-Pentanone, 4-...	4.869	26.8	ng	1639000	1	7.704	1225040	20.0
Oleic Acid	19.227	2.1	ng	260581	5	21.297	2491890	20.0
unknown21.785	21.785	8.5	ng	1059640	5	21.297	2491890	20.0
unknown21.839	21.839	21.7	ng	2708590	5	21.297	2491890	20.0